



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 05:36 am BST

PDB ID : 6QL9  
Title : Structure of Fatty acid synthase complex from *Saccharomyces cerevisiae* at 2.9 Angstrom  
Authors : Singh, K.; Graf, B.; Linden, A.; Sautner, V.; Urlaub, H.; Tittmann, K.; Stark, H.; Chari, A.  
Deposited on : 2019-01-31  
Resolution : 2.82 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

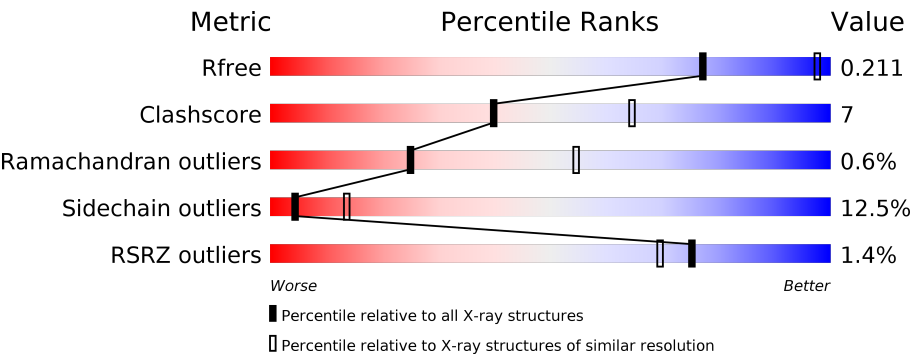
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1887	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>73%18%• 7%</div></div>
1	B	1887	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>73%17%• 7%</div></div>
1	C	1887	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>73%18%• 7%</div></div>
1	D	1887	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>73%17%• 6%</div></div>
1	E	1887	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>72%18%• 7%</div></div>
1	F	1887	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>73%17%• 7%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	2051	
2	J	2051	
3	H	2051	
3	I	2051	
3	K	2051	
3	L	2051	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MLI	J	2102	-	-	X	-
6	NA	C	1914	-	-	-	X
7	A2P	A	1918	-	-	-	X
7	A2P	B	1918	-	-	-	X
7	A2P	E	1917	-	-	-	X
7	A2P	F	1912	-	-	-	X
8	ACT	B	1902	-	-	-	X
8	ACT	C	1903	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 179453 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1760	Total	C	N	O	S	0	0	0
			13686	8661	2308	2665	52			
1	B	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			
1	C	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			
1	D	1765	Total	C	N	O	S	0	0	0
			13729	8688	2314	2675	52			
1	E	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			
1	F	1759	Total	C	N	O	S	0	0	0
			13680	8658	2307	2663	52			

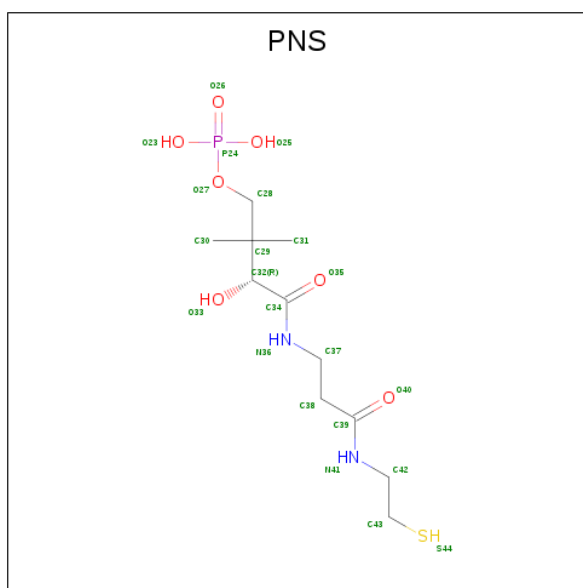
- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2036	Total	C	N	O	S	0	1	0
			16028	10271	2666	3035	56			
2	J	2035	Total	C	N	O	S	0	1	0
			16025	10272	2665	3032	56			

- Molecule 3 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	2035	Total	C	N	O	S	0	1	0
			16028	10274	2664	3034	56			
3	I	2034	Total	C	N	O	S	0	1	0
			16019	10266	2664	3033	56			
3	K	2035	Total	C	N	O	S	0	0	0
			16021	10269	2662	3034	56			
3	L	2036	Total	C	N	O	S	0	1	0
			16040	10280	2666	3038	56			

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula:  $C_{11}H_{23}N_2O_7PS$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 21	C 11	N 2	O 6	P 1	S 1	0	0
4	B	1	Total 21	C 11	N 2	O 6	P 1	S 1	0	0
4	C	1	Total 21	C 11	N 2	O 6	P 1	S 1	0	0
4	D	1	Total 21	C 11	N 2	O 6	P 1	S 1	0	0
4	E	1	Total 21	C 11	N 2	O 6	P 1	S 1	0	0
4	F	1	Total 21	C 11	N 2	O 6	P 1	S 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	F	1	Total 4	C 2	O 2	0	0
5	H	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0
5	J	1	Total 4	C 2	O 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

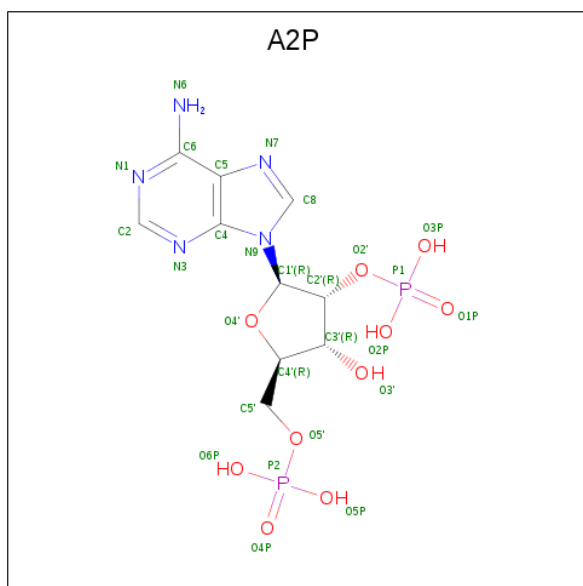
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	2	Total 2	Na 2	0	0
6	J	2	Total 2	Na 2	0	0
6	D	8	Total 8	Na 8	0	0
6	K	2	Total 2	Na 2	0	0
6	E	3	Total 3	Na 3	0	0
6	H	2	Total 2	Na 2	0	0
6	B	5	Total 5	Na 5	0	0
6	I	1	Total 1	Na 1	0	0

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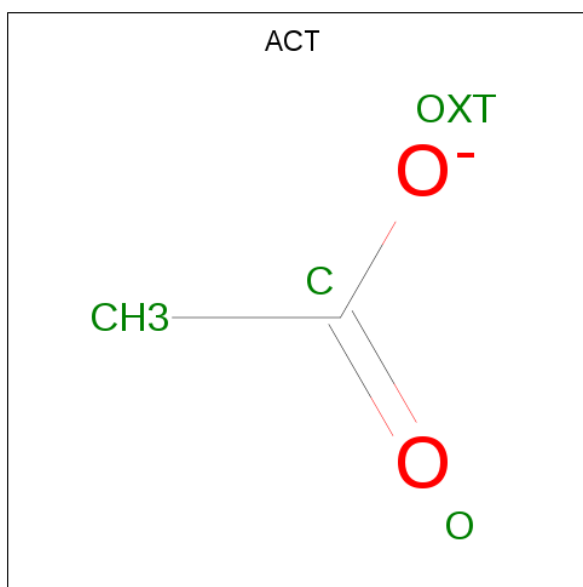
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	4	Total	Na	0	0
			4	4		
6	A	6	Total	Na	0	0
			6	6		
6	L	2	Total	Na	0	0
			2	2		
6	F	2	Total	Na	0	0
			2	2		

- Molecule 7 is ADENOSINE-2'-5'-DIPHOSPHATE (three-letter code: A2P) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



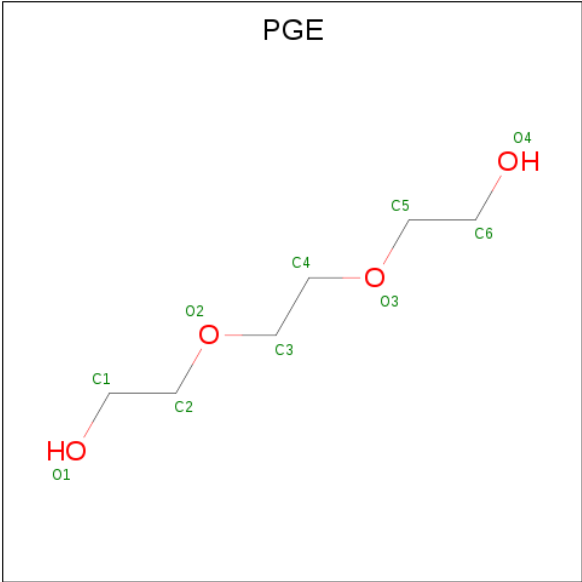
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



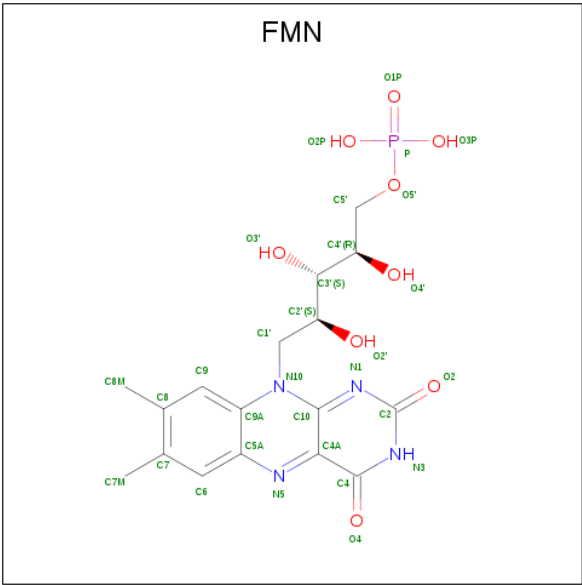
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	1	Total	C	O		0	0
			10	6	4			

- Molecule 10 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



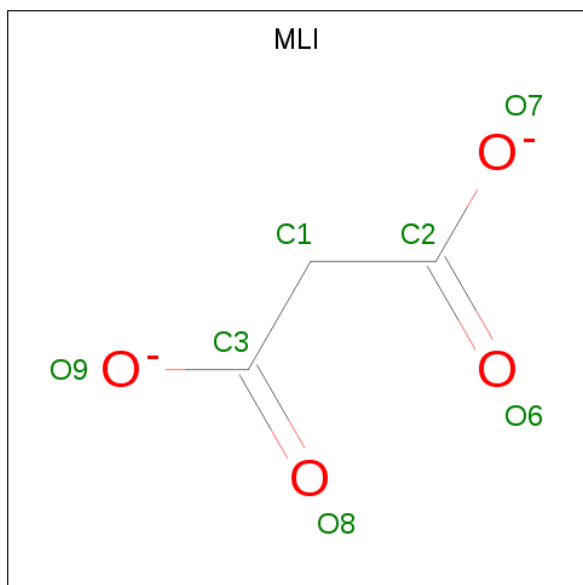
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	J	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	K	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
10	L	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 11 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	G	1	Total	C	O	0	0
			7	3	4		
11	J	1	Total	C	O	0	0
			7	3	4		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	42	Total	O	0	0
			42	42		
12	B	36	Total	O	0	0
			36	36		
12	C	42	Total	O	0	0
			42	42		
12	D	60	Total	O	0	0
			60	60		

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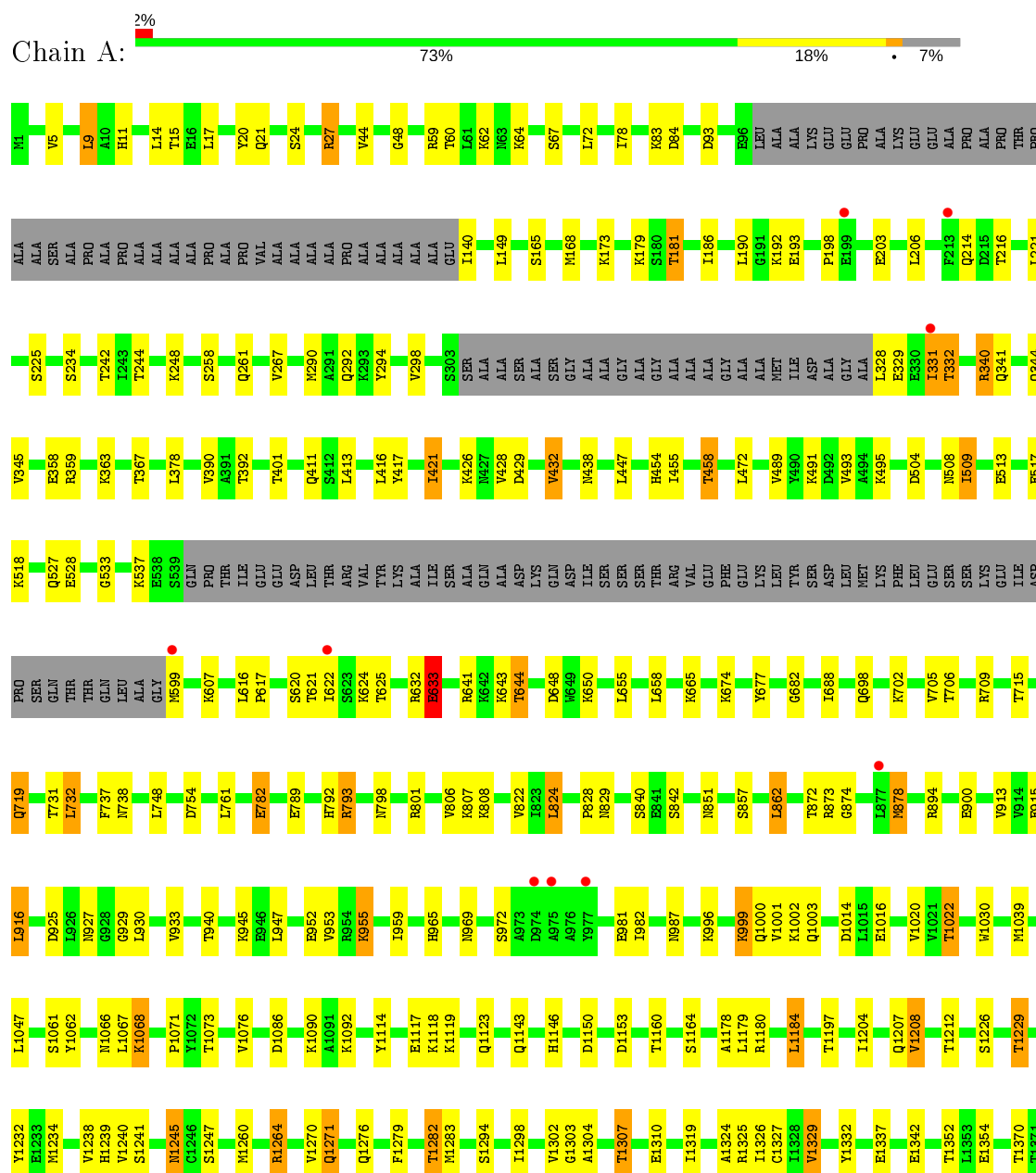
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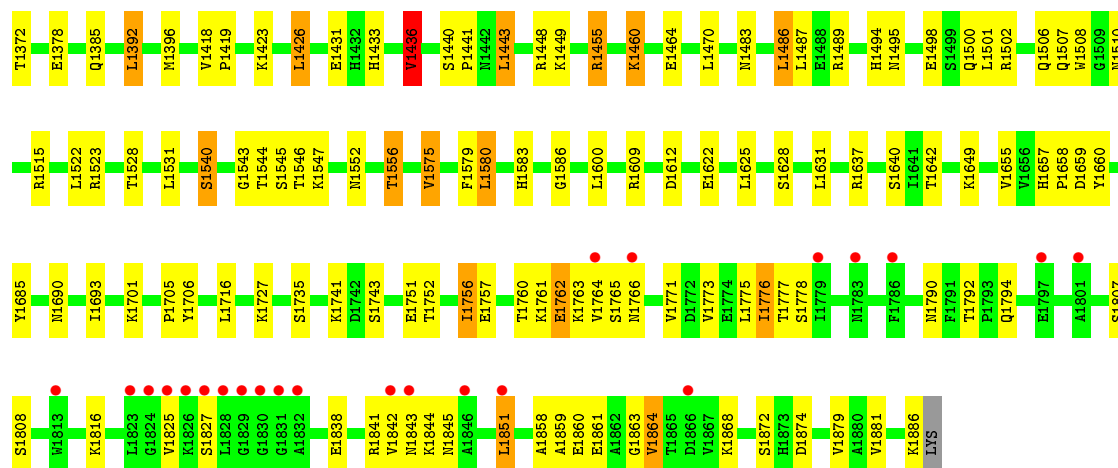
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	30	Total 30	O 30	0	0
12	F	24	Total 24	O 24	0	0
12	G	19	Total 19	O 19	0	0
12	H	24	Total 24	O 24	0	0
12	I	17	Total 17	O 17	0	0
12	J	17	Total 17	O 17	0	0
12	K	5	Total 5	O 5	0	0
12	L	12	Total 12	O 12	0	0

### 3 Residue-property plots

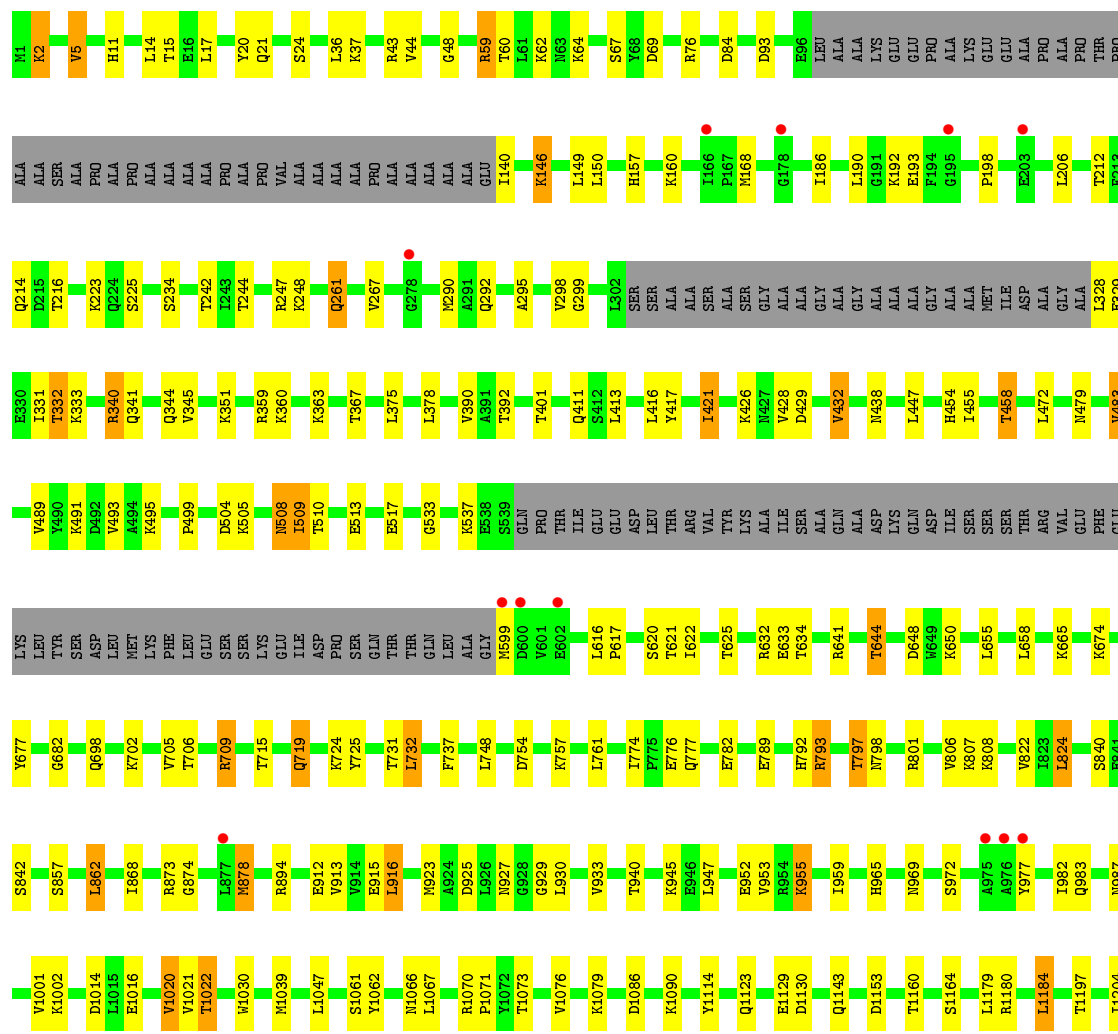
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fatty acid synthase subunit alpha

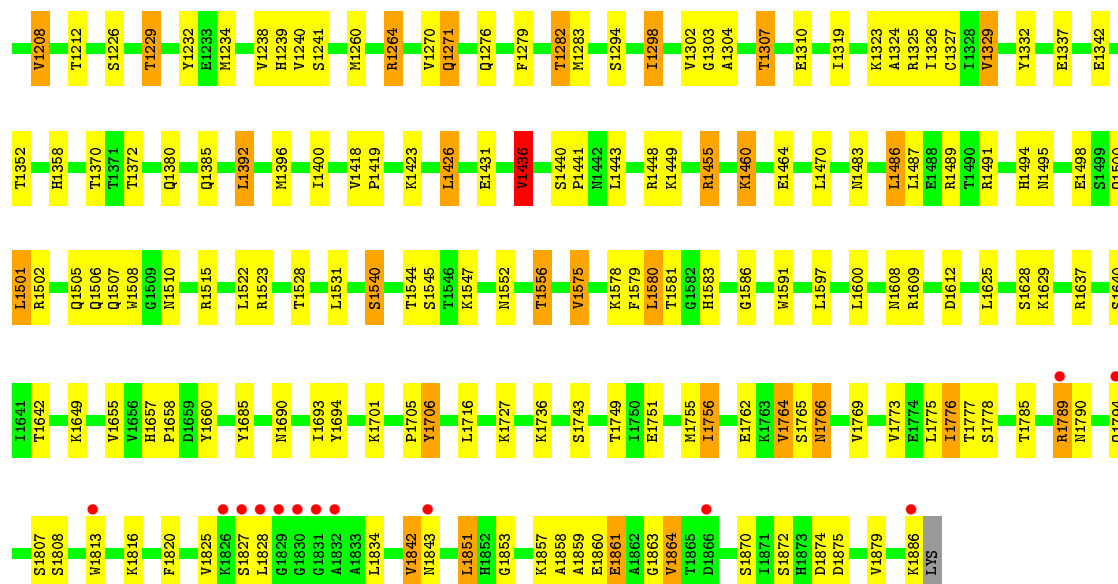




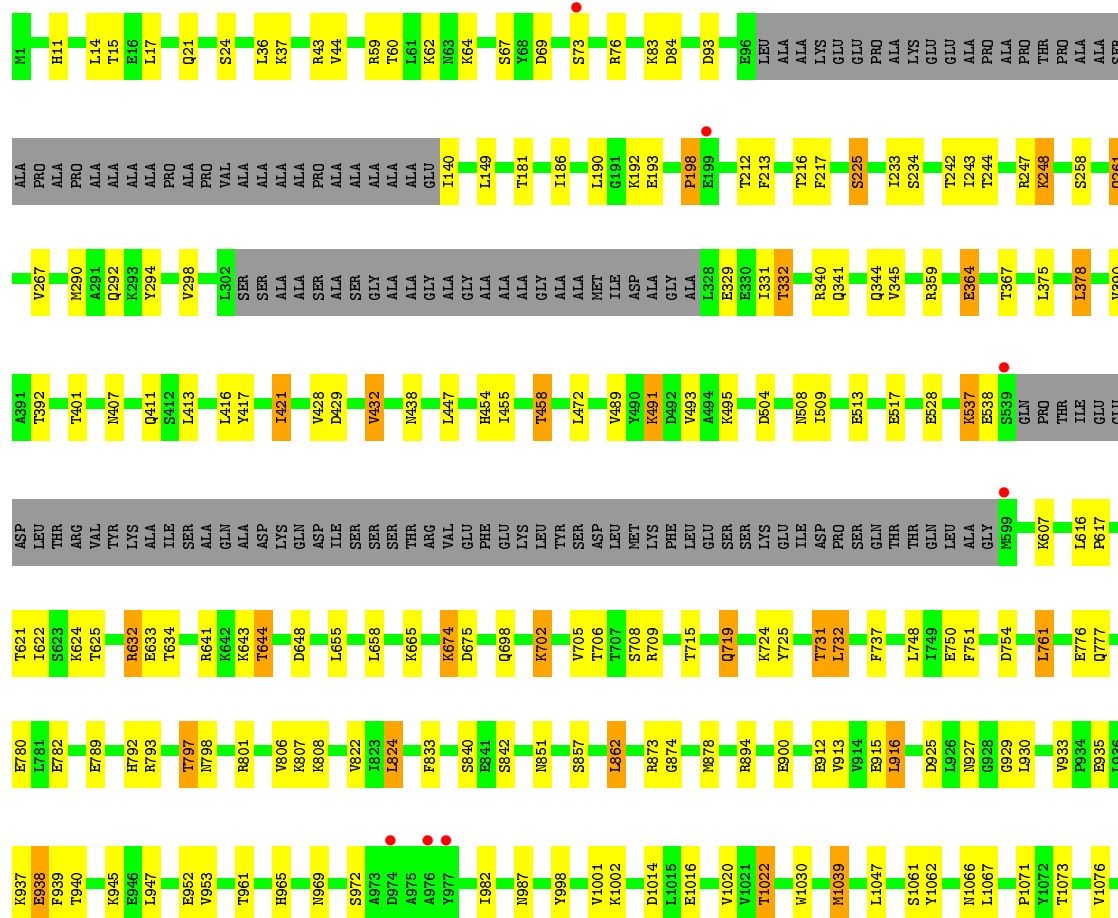
• Molecule 1: Fatty acid synthase subunit alpha

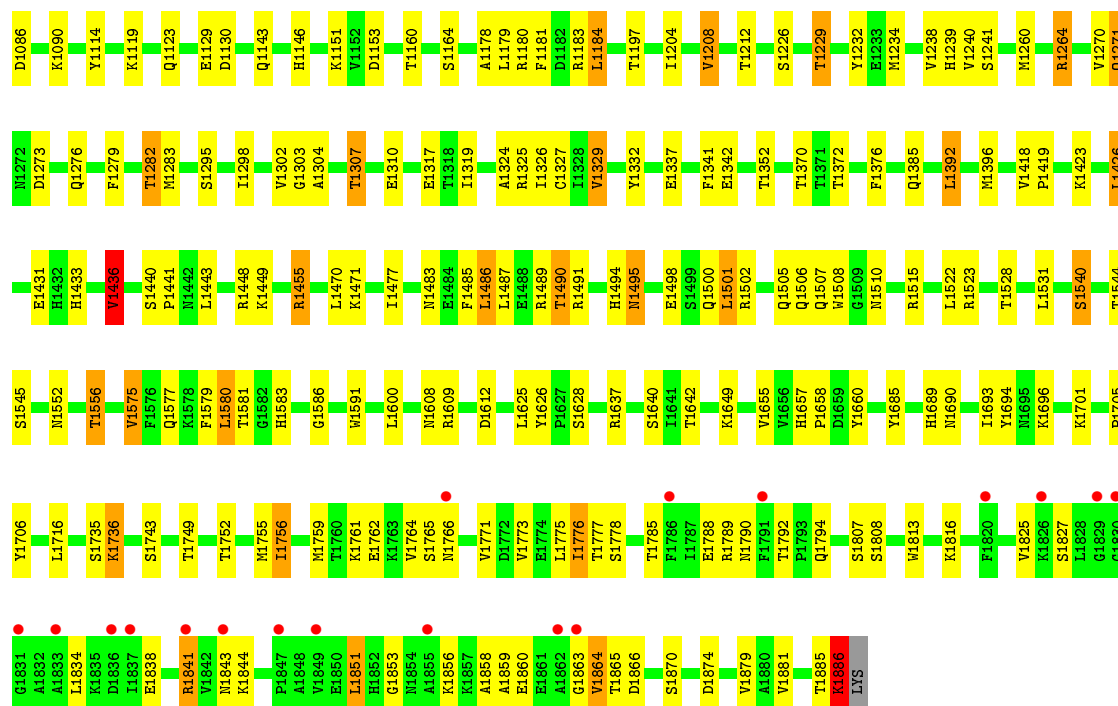




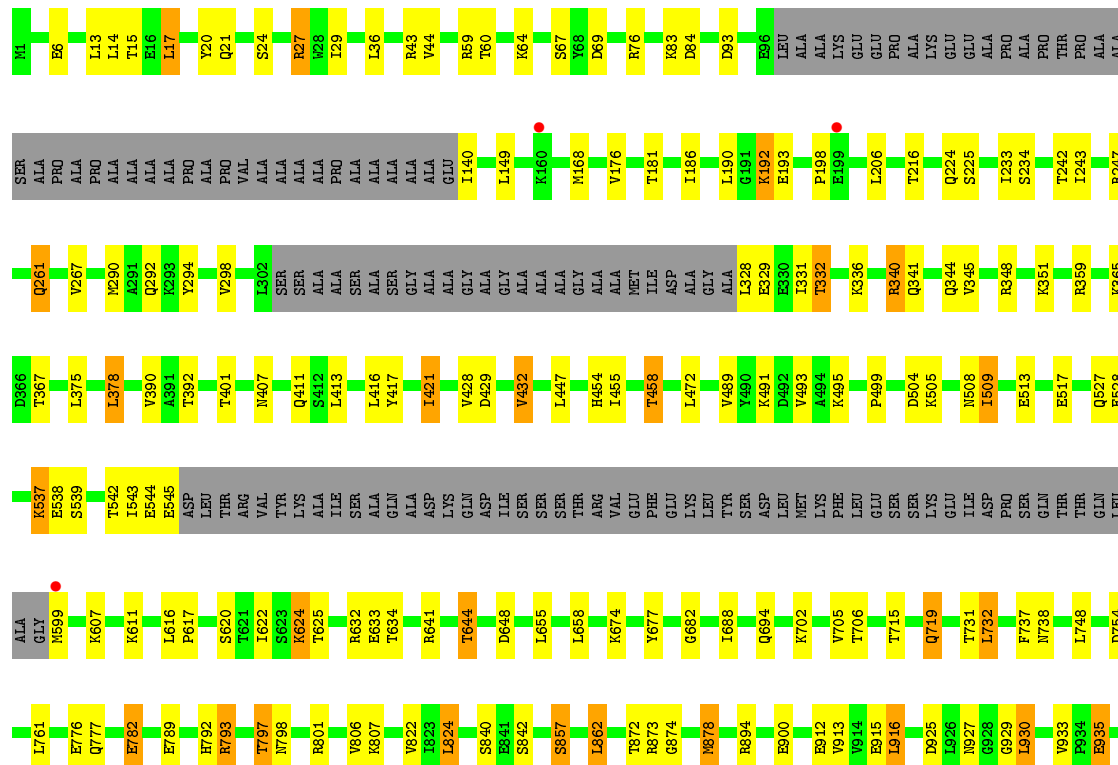


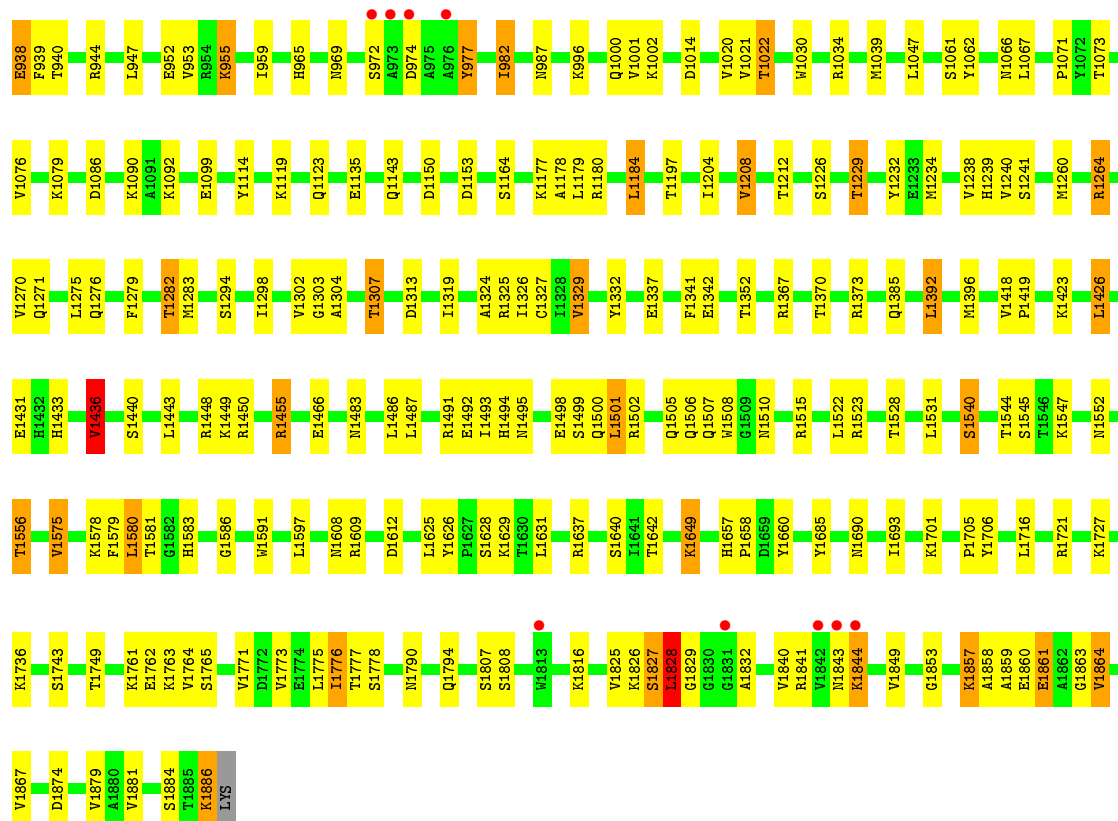
• Molecule 1: Fatty acid synthase subunit alpha



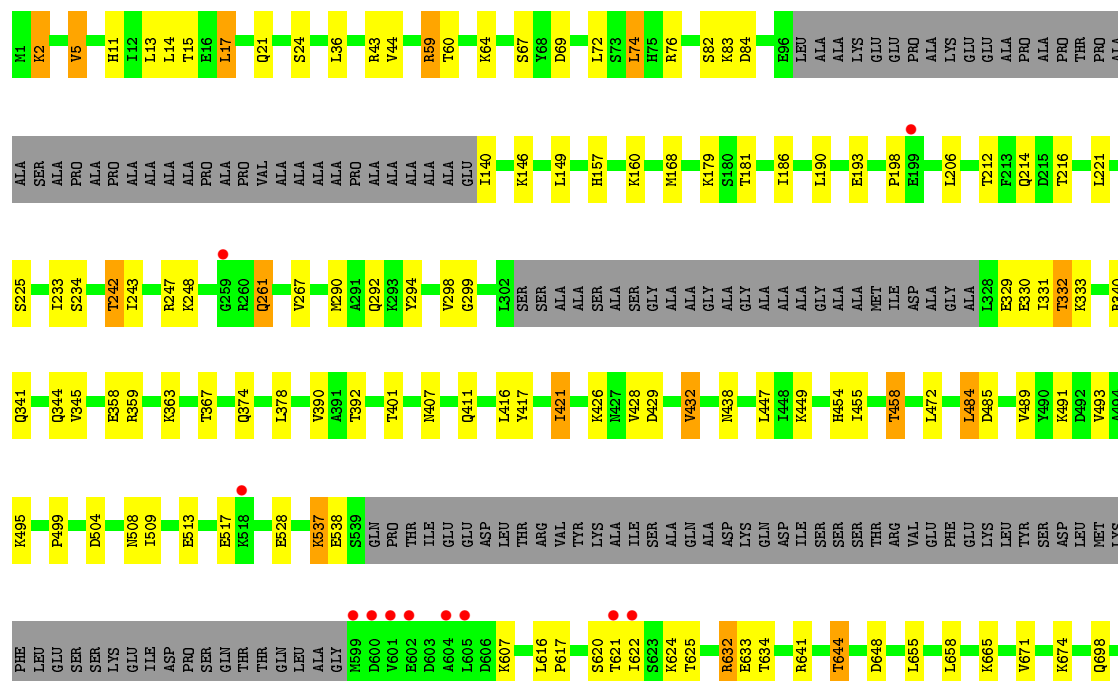
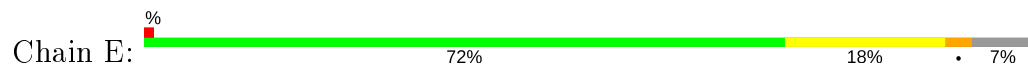


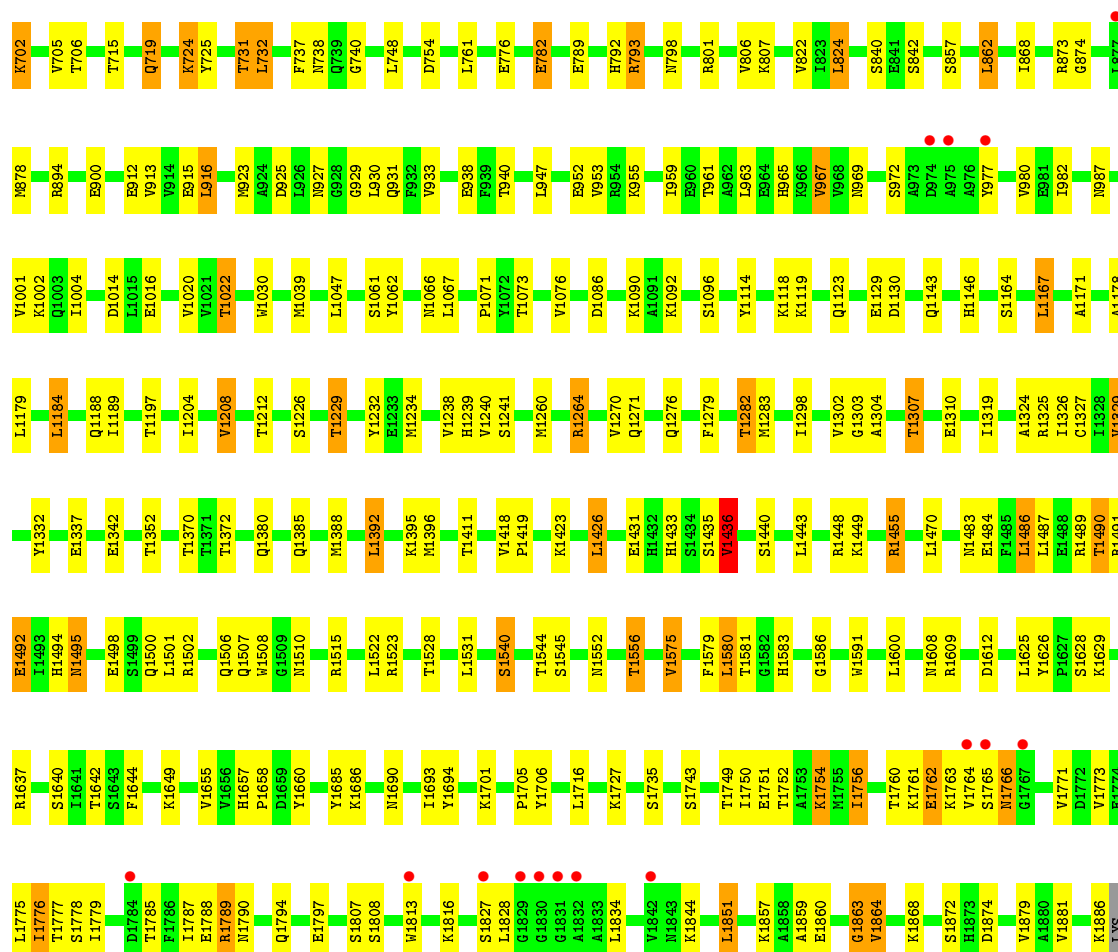
● Molecule 1: Fatty acid synthase subunit alpha



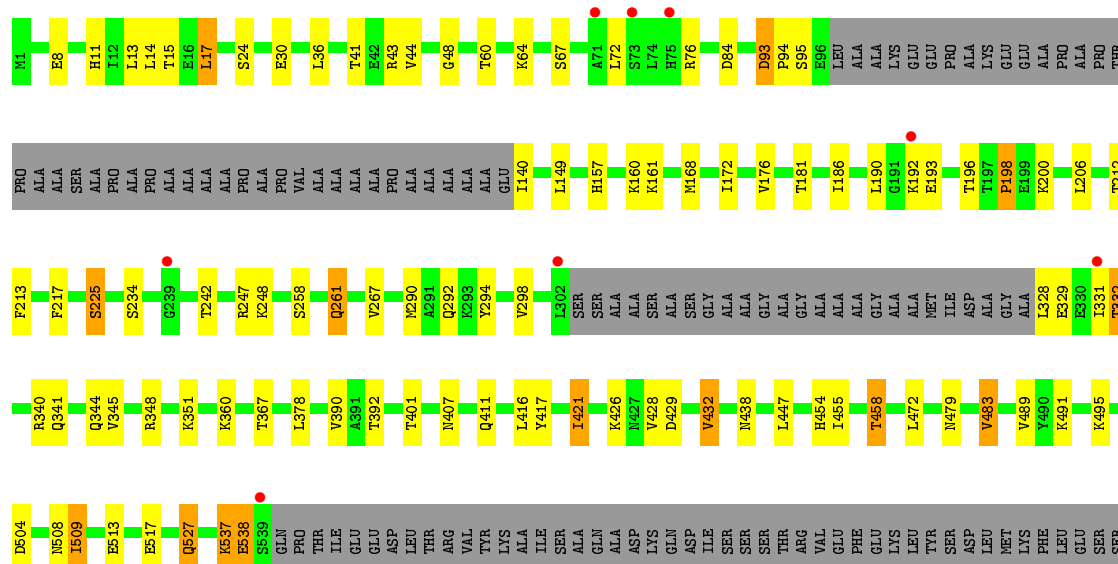
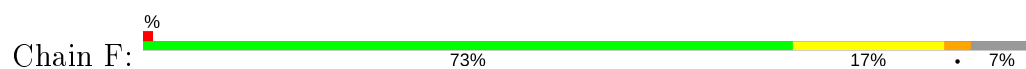


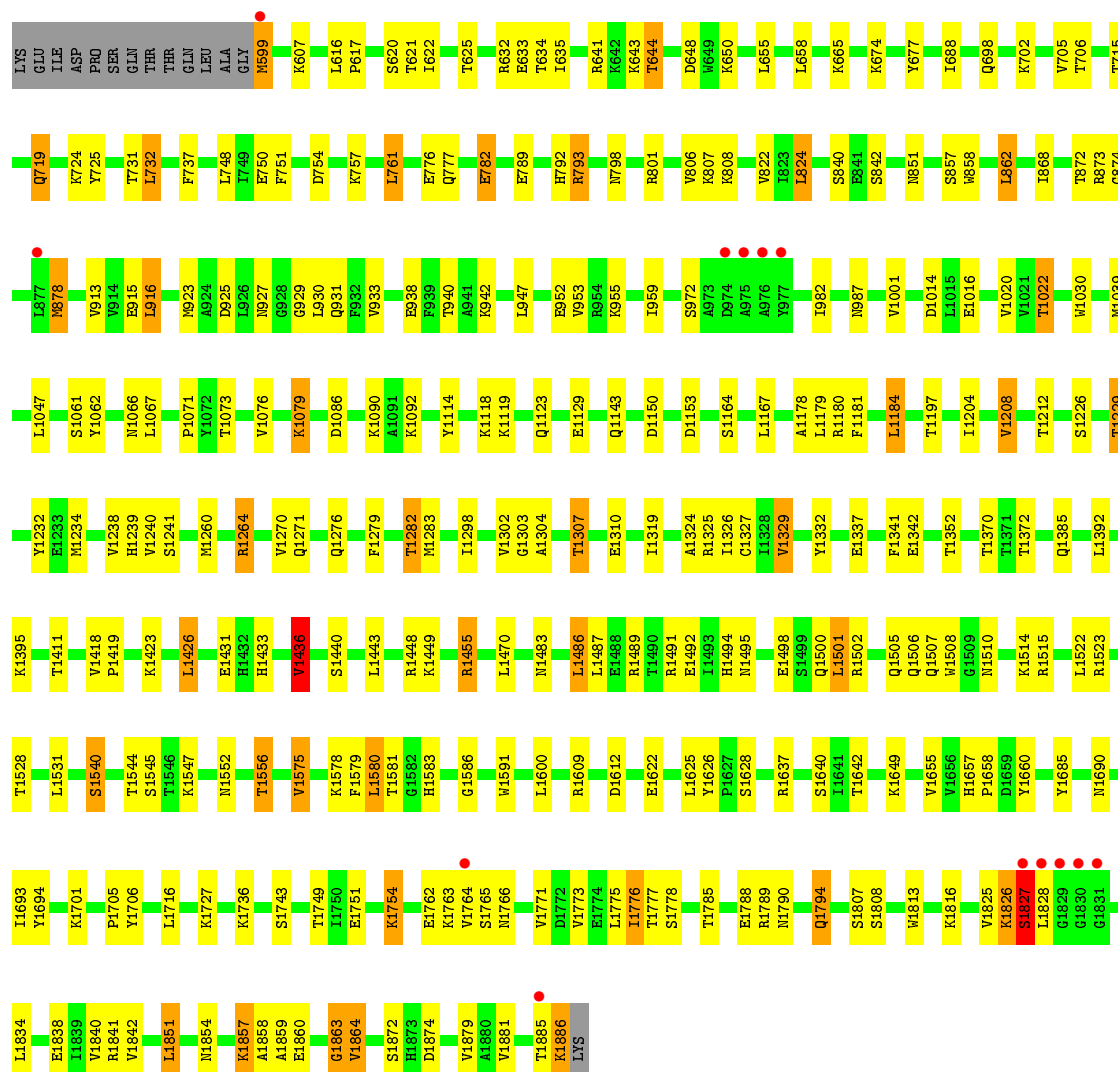
• Molecule 1: Fatty acid synthase subunit alpha



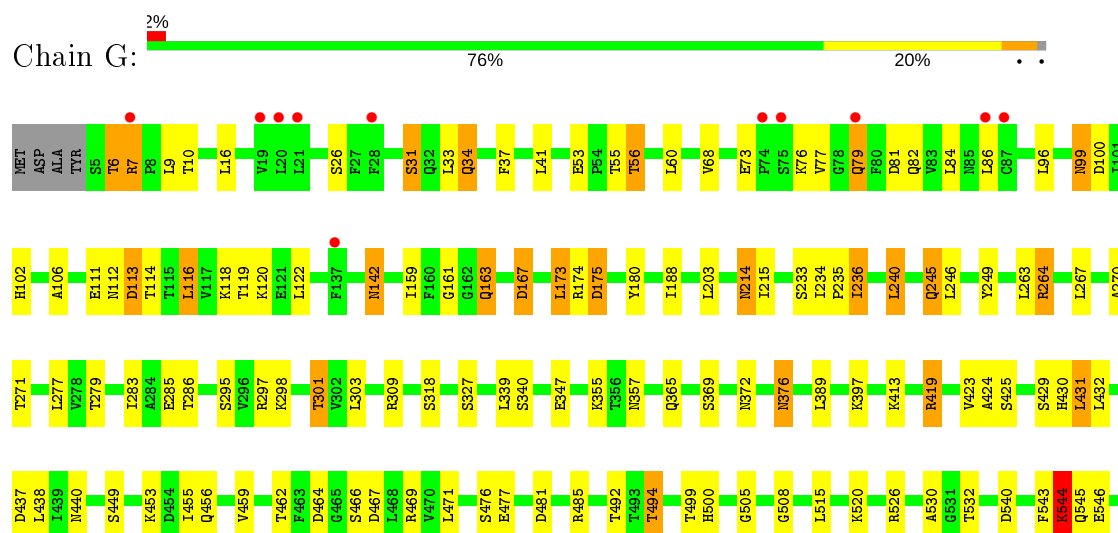


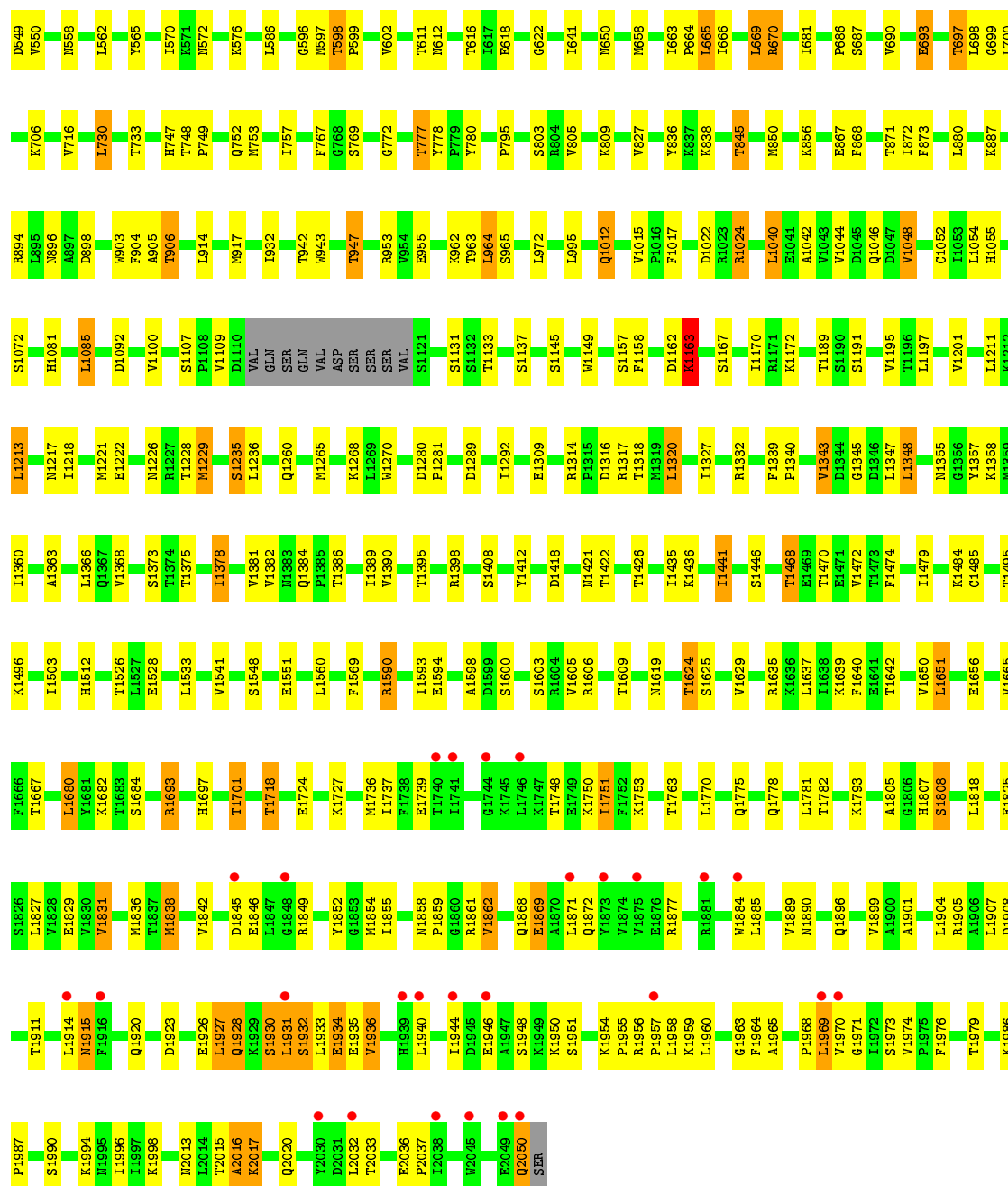
• Molecule 1: Fatty acid synthase subunit alpha



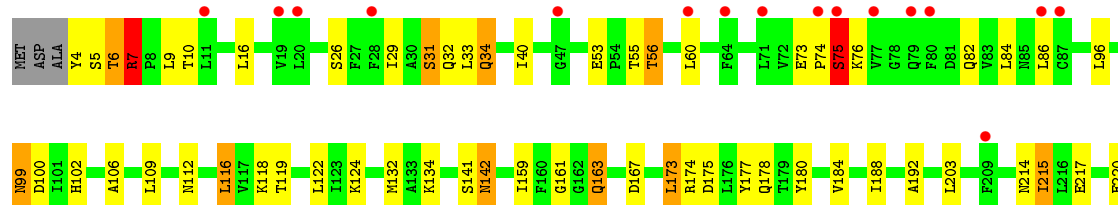
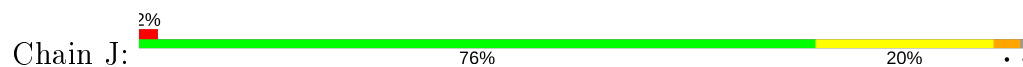


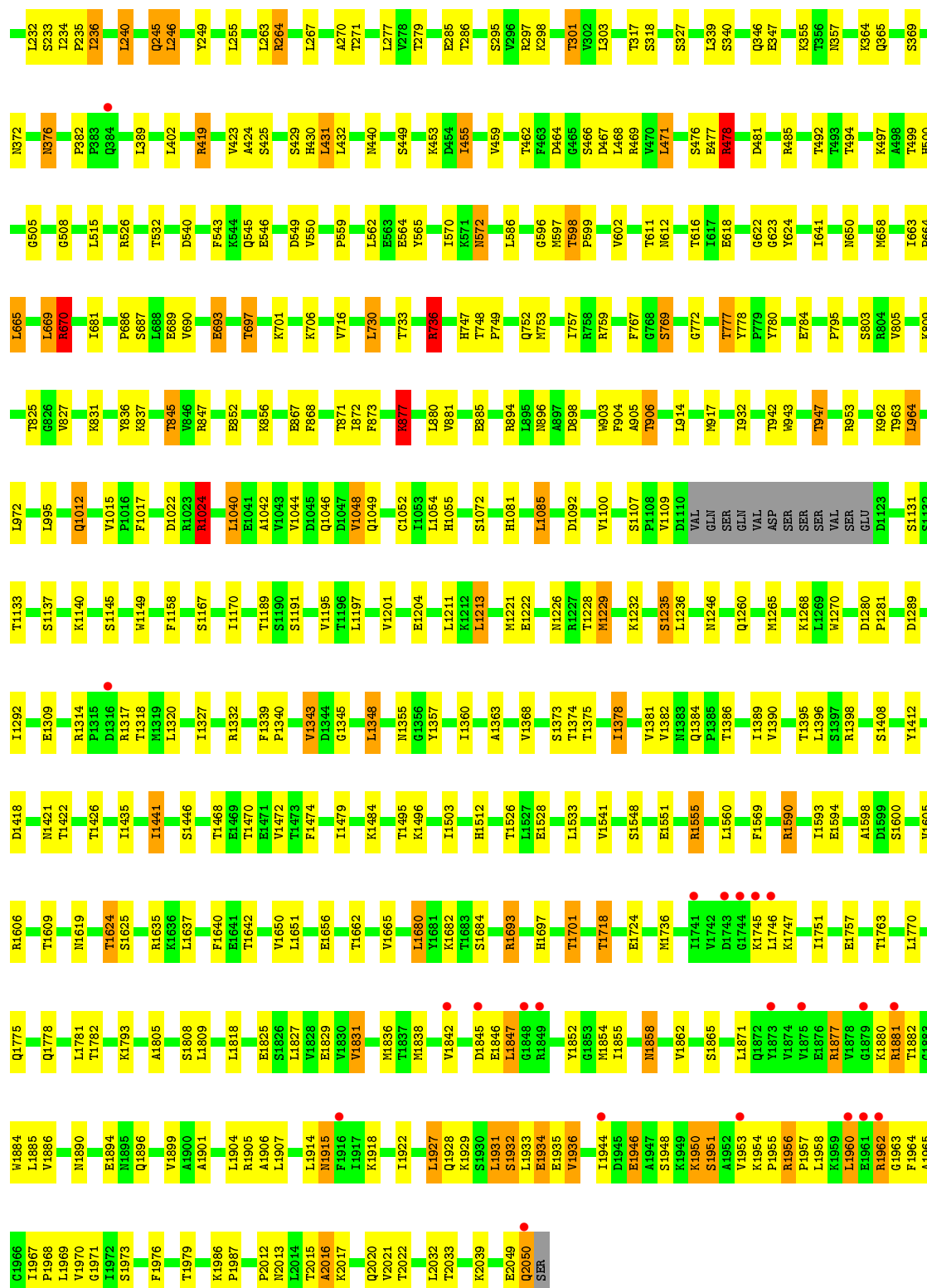
• Molecule 2: Fatty acid synthase subunit beta





• Molecule 2: Fatty acid synthase subunit beta

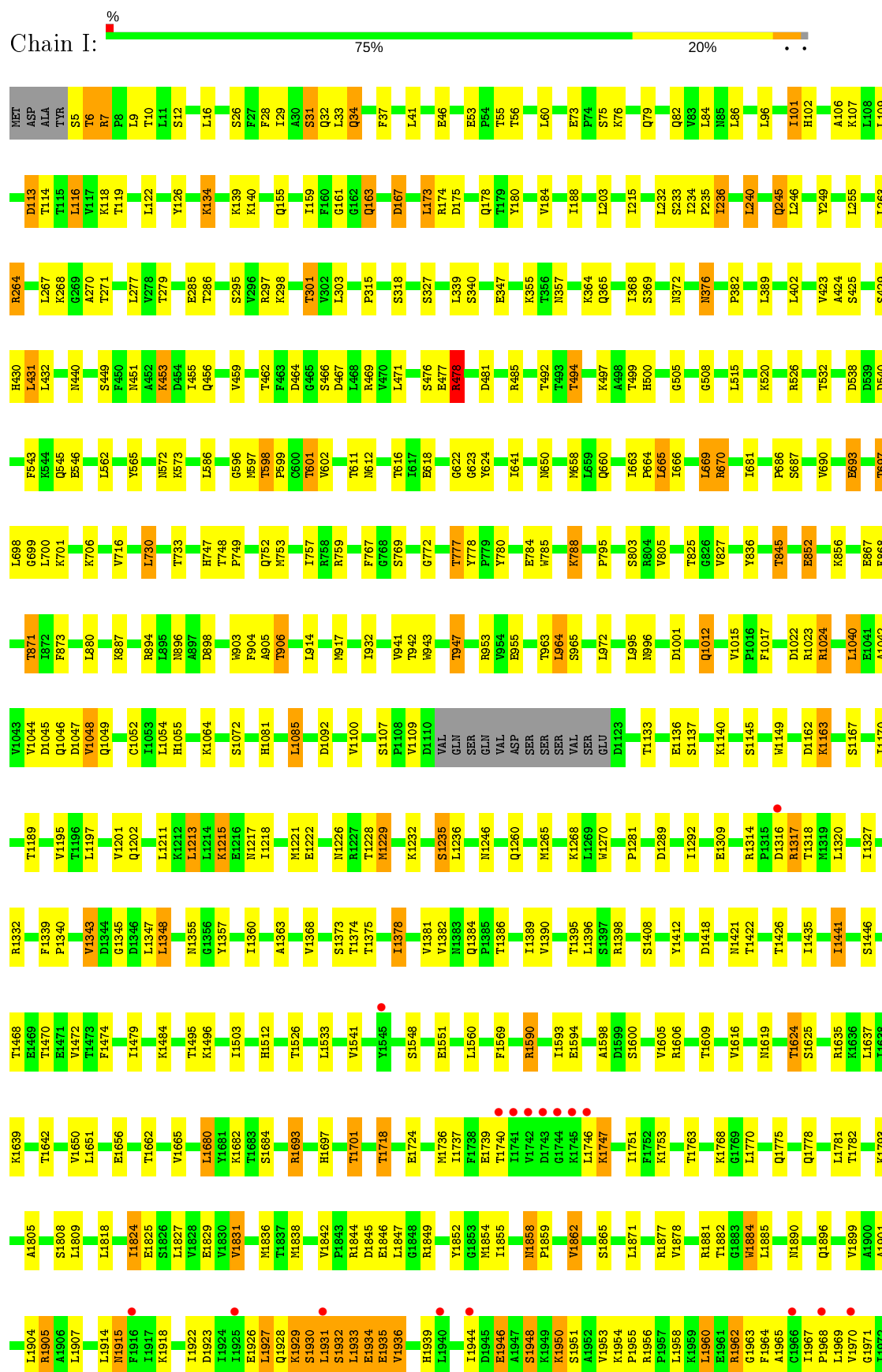


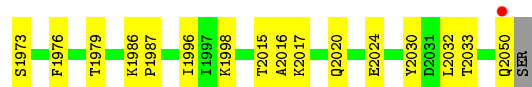




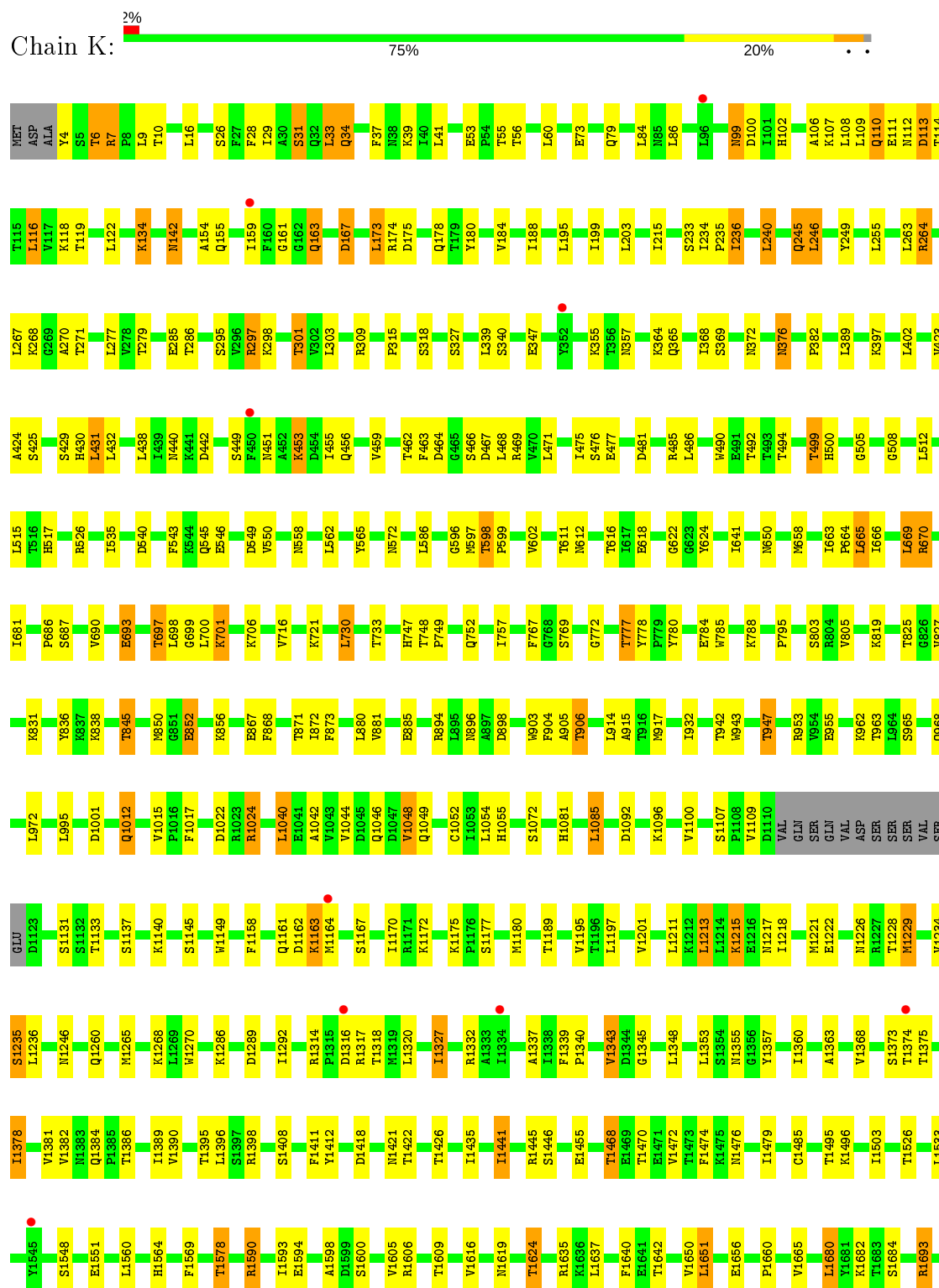


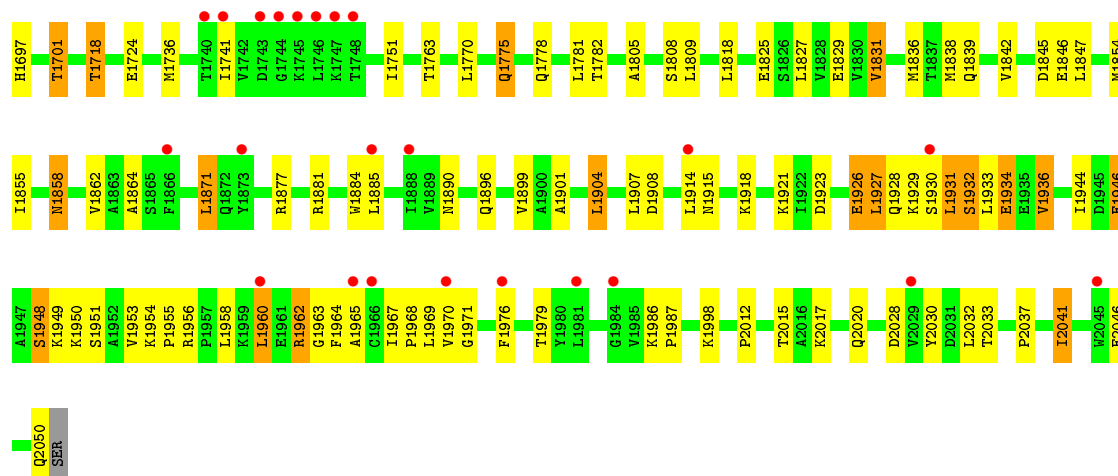
• Molecule 3: Fatty acid synthase subunit beta



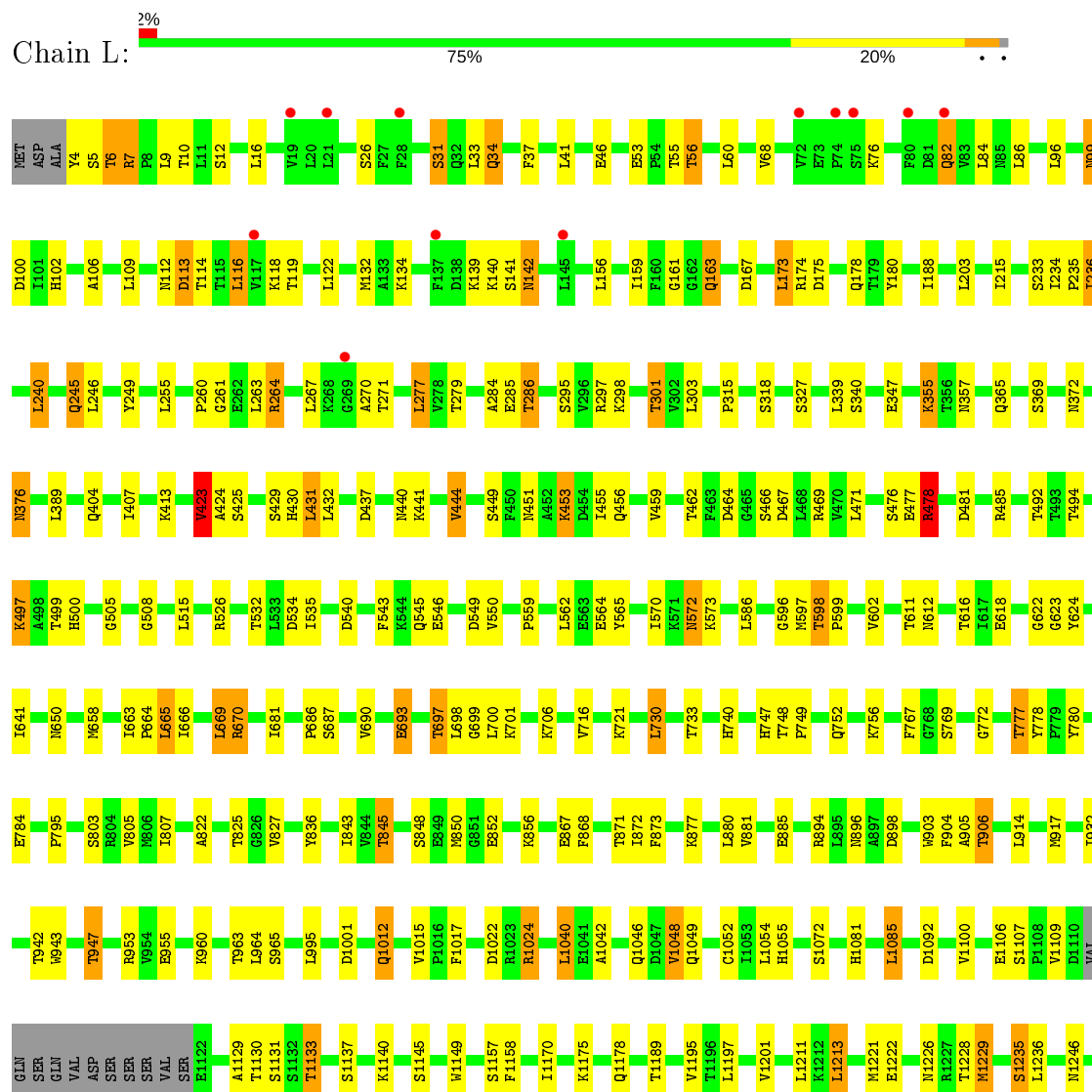


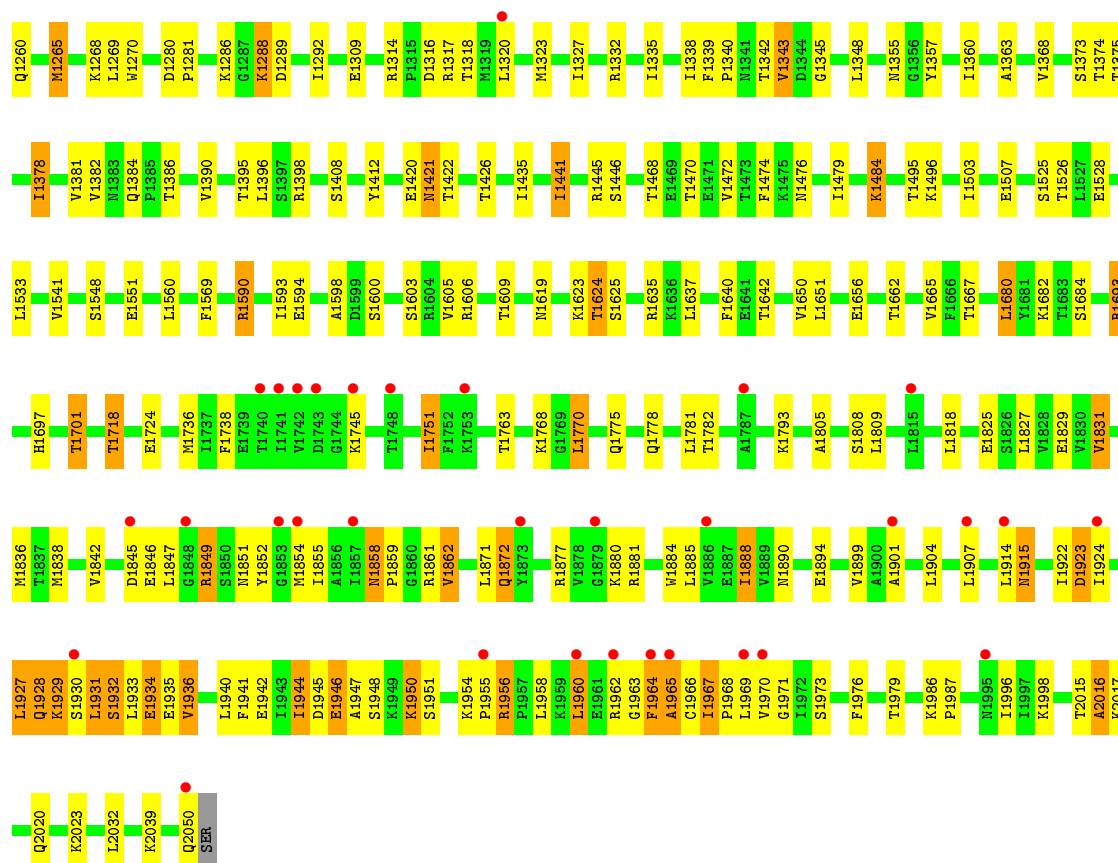
• Molecule 3: Fatty acid synthase subunit beta





• Molecule 3: Fatty acid synthase subunit beta





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.62Å 347.60Å 265.27Å 90.00° 107.88° 90.00°	Depositor
Resolution (Å)	191.50 – 2.82 204.26 – 2.82	Depositor EDS
% Data completeness (in resolution range)	78.6 (191.50-2.82) 78.6 (204.26-2.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.192 , 0.211 0.194 , 0.211	Depositor DCC
$R_{free}$ test set	35171 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.8	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	179453	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A2P, PGE, J8W, NA, PNS, MLI, EDO, FMN, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.68	2/13939 (0.0%)	0.85	5/18837 (0.0%)
1	B	0.69	0/13933	0.85	4/18829 (0.0%)
1	C	0.69	1/13933 (0.0%)	0.84	3/18829 (0.0%)
1	D	0.69	0/13983	0.86	8/18898 (0.0%)
1	E	0.69	1/13933 (0.0%)	0.85	2/18829 (0.0%)
1	F	0.68	0/13933	0.83	2/18829 (0.0%)
2	G	0.67	0/16394	0.82	1/22244 (0.0%)
2	J	0.67	0/16392	0.83	4/22242 (0.0%)
3	H	0.67	1/16385 (0.0%)	0.82	0/22231
3	I	0.67	0/16372	0.82	1/22213 (0.0%)
3	K	0.67	0/16374	0.82	0/22216
3	L	0.67	0/16394	0.81	3/22243 (0.0%)
All	All	0.68	5/181965 (0.0%)	0.83	33/246440 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	D	0	1
3	I	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1484	GLU	CD-OE2	6.00	1.32	1.25
3	H	852	GLU	CD-OE1	5.37	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1354	GLU	CD-OE1	5.29	1.31	1.25
1	A	1378	GLU	CD-OE1	5.19	1.31	1.25
1	C	1317	GLU	CD-OE1	5.05	1.31	1.25

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1886	LYS	CA-C-O	7.42	135.69	120.10
3	L	1964	PHE	CB-CA-C	7.13	124.66	110.40
1	E	1264	ARG	CG-CD-NE	-7.07	96.96	111.80
1	A	1264	ARG	CG-CD-NE	-7.04	97.01	111.80
1	B	1264	ARG	CG-CD-NE	-7.03	97.03	111.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1207	GLN	Peptide
1	C	1841	ARG	Peptide
1	C	538	GLU	Peptide
1	D	1828	LEU	Peptide
3	I	1844	ARG	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13686	0	13661	211	2
1	B	13680	0	13658	214	0
1	C	13680	0	13658	222	0
1	D	13729	0	13701	207	2
1	E	13680	0	13658	212	0
1	F	13680	0	13658	201	0
2	G	16028	0	15999	241	0
2	J	16025	0	15997	248	0
3	H	16028	0	15993	246	0
3	I	16019	0	15983	249	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	16021	0	15986	261	0
3	L	16040	0	15998	295	0
4	A	21	0	21	1	0
4	B	21	0	21	1	0
4	C	21	0	21	0	0
4	D	21	0	21	0	0
4	E	21	0	21	0	0
4	F	21	0	21	2	0
5	A	40	0	60	0	0
5	B	40	0	60	4	0
5	C	36	0	54	1	0
5	D	52	0	78	1	0
5	E	48	0	72	0	0
5	F	32	0	48	0	0
5	H	4	0	6	0	0
5	J	16	0	24	2	0
6	A	6	0	0	0	0
6	B	5	0	0	0	0
6	C	4	0	0	0	0
6	D	8	0	0	0	0
6	E	3	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
6	I	1	0	0	0	0
6	J	2	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0
7	A	27	0	11	3	0
7	B	27	0	11	5	0
7	C	27	0	11	2	0
7	D	27	0	11	3	0
7	E	27	0	11	2	0
7	F	27	0	11	1	0
8	B	4	0	3	1	0
8	C	8	0	6	2	0
8	H	12	0	9	0	0
9	E	10	0	14	0	0
10	G	31	0	19	4	0
10	H	31	0	19	4	0
10	I	31	0	19	5	0
10	J	31	0	19	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	31	0	19	5	0
10	L	31	0	19	5	0
11	G	7	0	2	1	0
11	J	7	0	2	2	0
12	A	42	0	0	1	0
12	B	36	0	0	0	0
12	C	42	0	0	0	0
12	D	60	0	0	1	0
12	E	30	0	0	0	0
12	F	24	0	0	1	0
12	G	19	0	0	1	0
12	H	24	0	0	2	0
12	I	17	0	0	1	0
12	J	17	0	0	0	0
12	K	5	0	0	0	0
12	L	12	0	0	0	0
All	All	179453	0	178694	2594	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 2594 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ASP:OD2	1:B:508:ASN:OD1	1.53	1.21
3:K:1904:LEU:HD22	3:K:1960:LEU:HD23	1.32	1.12
3:I:867:GLU:O	3:I:871:THR:OG1	1.69	1.08
1:C:1486:LEU:O	1:C:1490:THR:HG22	1.55	1.06
1:B:193:GLU:OE2	1:B:225:SER:OG	1.72	1.06

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1843:ASN:O	1:D:1843:ASN:O[1_655]	1.70	0.50
1:A:1845:ASN:OD1	1:D:1844:LYS:O[1_655]	1.96	0.24

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1752/1887 (93%)	1667 (95%)	77 (4%)	8 (0%)	29	59
1	B	1751/1887 (93%)	1663 (95%)	77 (4%)	11 (1%)	25	54
1	C	1751/1887 (93%)	1661 (95%)	80 (5%)	10 (1%)	25	54
1	D	1757/1887 (93%)	1664 (95%)	81 (5%)	12 (1%)	22	51
1	E	1751/1887 (93%)	1667 (95%)	75 (4%)	9 (0%)	29	59
1	F	1751/1887 (93%)	1662 (95%)	79 (4%)	10 (1%)	25	54
2	G	2033/2051 (99%)	1915 (94%)	105 (5%)	13 (1%)	25	54
2	J	2032/2051 (99%)	1914 (94%)	101 (5%)	17 (1%)	19	47
3	H	2031/2051 (99%)	1913 (94%)	105 (5%)	13 (1%)	25	54
3	I	2030/2051 (99%)	1911 (94%)	106 (5%)	13 (1%)	25	54
3	K	2030/2051 (99%)	1909 (94%)	109 (5%)	12 (1%)	25	54
3	L	2032/2051 (99%)	1912 (94%)	107 (5%)	13 (1%)	25	54
All	All	22701/23628 (96%)	21458 (94%)	1102 (5%)	141 (1%)	25	54

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1843	ASN
1	D	539	SER
1	F	1827	SER
2	G	7	ARG
2	G	1869	GLU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1484/1566 (95%)	1310 (88%)	174 (12%)	5	16
1	B	1483/1566 (95%)	1306 (88%)	177 (12%)	5	15
1	C	1483/1566 (95%)	1319 (89%)	164 (11%)	6	18
1	D	1489/1566 (95%)	1315 (88%)	174 (12%)	5	16
1	E	1483/1566 (95%)	1299 (88%)	184 (12%)	4	14
1	F	1483/1566 (95%)	1310 (88%)	173 (12%)	5	16
2	G	1776/1789 (99%)	1553 (87%)	223 (13%)	4	13
2	J	1775/1789 (99%)	1540 (87%)	235 (13%)	4	11
3	H	1774/1788 (99%)	1557 (88%)	217 (12%)	5	14
3	I	1773/1788 (99%)	1529 (86%)	244 (14%)	3	10
3	K	1773/1788 (99%)	1541 (87%)	232 (13%)	4	12
3	L	1775/1788 (99%)	1533 (86%)	242 (14%)	3	11
All	All	19551/20126 (97%)	17112 (88%)	2439 (12%)	4	14

5 of 2439 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	431	LEU
3	H	880	LEU
3	L	369	SER
2	G	809	LYS
2	G	1845	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 458 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1239	HIS
2	G	1928	GLN
3	L	376	ASN
1	F	1494	HIS
2	G	558	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	J8W	I	1808	3	7,11,12	2.22	1 (14%)	5,13,15	2.47	2 (40%)
3	J8W	L	1808	3	7,11,12	2.04	1 (14%)	5,13,15	2.63	2 (40%)
3	J8W	H	1808	3	7,11,12	1.95	1 (14%)	5,13,15	2.27	2 (40%)
3	J8W	K	1808	3	7,11,12	2.11	1 (14%)	5,13,15	2.55	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	J8W	I	1808	3	-	4/7/11/13	-
3	J8W	L	1808	3	-	4/7/11/13	-
3	J8W	H	1808	3	-	4/7/11/13	-
3	J8W	K	1808	3	-	4/7/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1808	J8W	OG-C2	5.59	1.49	1.33
3	K	1808	J8W	OG-C2	5.35	1.49	1.33
3	L	1808	J8W	OG-C2	5.16	1.48	1.33
3	H	1808	J8W	OG-C2	4.94	1.47	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1808	J8W	OG-C2-C1	4.29	118.34	111.07
3	K	1808	J8W	OG-C2-C1	3.85	117.60	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1808	J8W	OG-C2-C1	3.80	117.52	111.07
3	H	1808	J8W	CB-OG-C2	3.78	131.14	117.12
3	K	1808	J8W	CB-OG-C2	3.75	131.00	117.12

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1808	J8W	N-CA-CB-OG
3	I	1808	J8W	C-CA-CB-OG
3	L	1808	J8W	N-CA-CB-OG
3	L	1808	J8W	C-CA-CB-OG
3	H	1808	J8W	N-CA-CB-OG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1808	J8W	1	0
3	L	1808	J8W	1	0
3	H	1808	J8W	1	0
3	K	1808	J8W	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 133 ligands modelled in this entry, 39 are monoatomic - leaving 94 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	PGE	E	1918	-	9,9,9	0.23	0	8,8,8	0.16	0
7	A2P	D	1923	-	25,29,29	0.71	0	31,45,45	0.85	1 (3%)
5	EDO	E	1909	-	3,3,3	0.17	0	2,2,2	0.41	0
5	EDO	F	1905	-	3,3,3	0.19	0	2,2,2	0.41	0
10	FMN	H	2101	-	31,33,33	2.26	4 (12%)	40,50,50	2.36	10 (25%)
8	ACT	B	1902	-	1,3,3	5.32	1 (100%)	0,3,3	0.00	-
10	FMN	J	2101	-	31,33,33	2.24	5 (16%)	40,50,50	2.34	10 (25%)
7	A2P	A	1918	-	25,29,29	0.65	0	31,45,45	0.70	0
5	EDO	B	1909	-	3,3,3	0.30	0	2,2,2	0.45	0
5	EDO	C	1909	-	3,3,3	0.22	0	2,2,2	0.41	0
5	EDO	B	1905	-	3,3,3	0.07	0	2,2,2	0.25	0
10	FMN	L	2101	-	31,33,33	2.23	6 (19%)	40,50,50	2.30	11 (27%)
5	EDO	B	1908	-	3,3,3	0.13	0	2,2,2	0.29	0
5	EDO	J	2106	-	3,3,3	0.07	0	2,2,2	0.35	0
10	FMN	K	2101	-	31,33,33	2.50	7 (22%)	40,50,50	2.67	11 (27%)
5	EDO	A	1911	-	3,3,3	0.19	0	2,2,2	0.45	0
5	EDO	C	1911	-	3,3,3	0.43	0	2,2,2	0.50	0
8	ACT	C	1902	-	1,3,3	3.82	1 (100%)	0,3,3	0.00	-
5	EDO	B	1903	-	3,3,3	0.10	0	2,2,2	0.18	0
8	ACT	H	2103	-	1,3,3	5.12	1 (100%)	0,3,3	0.00	-
5	EDO	A	1904	-	3,3,3	0.13	0	2,2,2	0.29	0
5	EDO	J	2105	-	3,3,3	0.08	0	2,2,2	0.17	0
5	EDO	E	1908	-	3,3,3	0.10	0	2,2,2	0.29	0
5	EDO	B	1907	-	3,3,3	0.15	0	2,2,2	0.25	0
5	EDO	D	1913	-	3,3,3	0.13	0	2,2,2	0.07	0
5	EDO	C	1904	-	3,3,3	0.15	0	2,2,2	0.36	0
5	EDO	C	1910	-	3,3,3	0.11	0	2,2,2	0.23	0
5	EDO	A	1906	-	3,3,3	0.05	0	2,2,2	0.12	0
5	EDO	C	1906	-	3,3,3	0.32	0	2,2,2	0.57	0
4	PNS	B	1901	1	13,20,21	0.61	0	18,26,29	1.23	2 (11%)
5	EDO	B	1904	-	3,3,3	0.12	0	2,2,2	0.16	0
5	EDO	E	1907	-	3,3,3	0.13	0	2,2,2	0.28	0
8	ACT	C	1903	-	1,3,3	3.55	1 (100%)	0,3,3	0.00	-
5	EDO	E	1913	-	3,3,3	0.16	0	2,2,2	0.34	0
5	EDO	A	1903	-	3,3,3	0.27	0	2,2,2	0.48	0
5	EDO	D	1905	-	3,3,3	0.11	0	2,2,2	0.13	0
5	EDO	A	1907	-	3,3,3	0.20	0	2,2,2	0.31	0
4	PNS	E	1901	1	13,20,21	0.64	0	18,26,29	1.21	1 (5%)
5	EDO	B	1911	-	3,3,3	0.18	0	2,2,2	0.39	0
5	EDO	D	1910	-	3,3,3	0.13	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	D	1903	-	3,3,3	0.32	0	2,2,2	0.51	0
5	EDO	F	1908	-	3,3,3	0.09	0	2,2,2	0.23	0
5	EDO	F	1903	-	3,3,3	0.10	0	2,2,2	0.20	0
8	ACT	H	2102	-	1,3,3	4.95	1 (100%)	0,3,3	0.00	-
5	EDO	B	1912	-	3,3,3	0.11	0	2,2,2	0.22	0
5	EDO	E	1910	-	3,3,3	0.15	0	2,2,2	0.36	0
5	EDO	E	1902	-	3,3,3	0.09	0	2,2,2	0.23	0
5	EDO	F	1902	-	3,3,3	0.09	0	2,2,2	0.13	0
5	EDO	J	2103	-	3,3,3	0.08	0	2,2,2	0.14	0
7	A2P	F	1912	-	25,29,29	0.69	0	31,45,45	0.75	1 (3%)
5	EDO	D	1912	-	3,3,3	0.11	0	2,2,2	0.23	0
5	EDO	D	1911	-	3,3,3	0.19	0	2,2,2	0.32	0
5	EDO	B	1906	-	3,3,3	0.16	0	2,2,2	0.49	0
5	EDO	E	1905	-	3,3,3	0.12	0	2,2,2	0.36	0
5	EDO	D	1914	-	3,3,3	0.24	0	2,2,2	0.45	0
5	EDO	C	1908	-	3,3,3	0.29	0	2,2,2	0.55	0
7	A2P	C	1917	-	25,29,29	0.73	0	31,45,45	0.80	1 (3%)
4	PNS	F	1901	1	13,20,21	0.86	0	18,26,29	2.65	7 (38%)
5	EDO	F	1907	-	3,3,3	0.13	0	2,2,2	0.33	0
5	EDO	C	1912	-	3,3,3	0.29	0	2,2,2	0.64	0
5	EDO	B	1910	-	3,3,3	0.15	0	2,2,2	0.33	0
5	EDO	D	1904	-	3,3,3	0.11	0	2,2,2	0.29	0
5	EDO	J	2104	-	3,3,3	0.10	0	2,2,2	0.34	0
5	EDO	E	1912	-	3,3,3	0.09	0	2,2,2	0.14	0
5	EDO	A	1908	-	3,3,3	0.10	0	2,2,2	0.28	0
4	PNS	C	1901	1	13,20,21	0.61	0	18,26,29	1.15	1 (5%)
4	PNS	A	1901	1	13,20,21	0.68	0	18,26,29	1.03	1 (5%)
5	EDO	C	1905	-	3,3,3	0.18	0	2,2,2	0.39	0
5	EDO	F	1904	-	3,3,3	0.31	0	2,2,2	0.49	0
5	EDO	E	1904	-	3,3,3	0.07	0	2,2,2	0.20	0
5	EDO	E	1906	-	3,3,3	0.05	0	2,2,2	0.10	0
5	EDO	A	1910	-	3,3,3	0.37	0	2,2,2	0.63	0
5	EDO	D	1907	-	3,3,3	0.13	0	2,2,2	0.32	0
5	EDO	D	1902	-	3,3,3	0.17	0	2,2,2	0.49	0
10	FMN	G	2101	-	31,33,33	2.17	6 (19%)	40,50,50	2.35	13 (32%)
11	MLI	G	2102	-	0,6,6	0.00	-	0,7,7	0.00	-
5	EDO	H	2105	-	3,3,3	0.11	0	2,2,2	0.18	0
5	EDO	A	1902	-	3,3,3	0.18	0	2,2,2	0.41	0
5	EDO	E	1903	-	3,3,3	0.13	0	2,2,2	0.24	0
4	PNS	D	1901	1	13,20,21	0.60	0	18,26,29	1.08	1 (5%)
5	EDO	D	1908	-	3,3,3	0.10	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	D	1909	-	3,3,3	0.28	0	2,2,2	0.64	0
5	EDO	C	1907	-	3,3,3	0.10	0	2,2,2	0.21	0
5	EDO	E	1911	-	3,3,3	0.19	0	2,2,2	0.41	0
11	MLI	J	2102	-	0,6,6	0.00	-	0,7,7	0.00	-
5	EDO	D	1906	-	3,3,3	0.43	0	2,2,2	0.65	0
8	ACT	H	2104	-	1,3,3	4.79	1 (100%)	0,3,3	0.00	-
5	EDO	A	1905	-	3,3,3	0.29	0	2,2,2	0.48	0
5	EDO	A	1909	-	3,3,3	0.32	0	2,2,2	0.51	0
5	EDO	F	1909	-	3,3,3	0.23	0	2,2,2	0.52	0
7	A2P	E	1917	-	25,29,29	0.68	0	31,45,45	0.81	1 (3%)
10	FMN	I	2101	-	31,33,33	2.08	5 (16%)	40,50,50	2.32	10 (25%)
5	EDO	F	1906	-	3,3,3	0.23	0	2,2,2	0.38	0
7	A2P	B	1918	-	25,29,29	0.70	0	31,45,45	0.96	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PGE	E	1918	-	-	3/7/7/7	-
7	A2P	D	1923	-	-	4/11/31/31	0/3/3/3
5	EDO	E	1909	-	-	1/1/1/1	-
5	EDO	F	1905	-	-	1/1/1/1	-
10	FMN	H	2101	-	-	2/18/18/18	0/3/3/3
10	FMN	J	2101	-	-	5/18/18/18	0/3/3/3
7	A2P	A	1918	-	-	5/11/31/31	0/3/3/3
5	EDO	B	1909	-	-	0/1/1/1	-
5	EDO	C	1909	-	-	1/1/1/1	-
5	EDO	B	1905	-	-	0/1/1/1	-
10	FMN	L	2101	-	-	3/18/18/18	0/3/3/3
5	EDO	B	1908	-	-	0/1/1/1	-
5	EDO	J	2106	-	-	1/1/1/1	-
10	FMN	K	2101	-	-	3/18/18/18	0/3/3/3
5	EDO	A	1911	-	-	1/1/1/1	-
5	EDO	C	1911	-	-	1/1/1/1	-
5	EDO	B	1903	-	-	1/1/1/1	-
5	EDO	A	1904	-	-	0/1/1/1	-
5	EDO	J	2105	-	-	0/1/1/1	-
5	EDO	E	1908	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	1907	-	-	0/1/1/1	-
5	EDO	D	1913	-	-	0/1/1/1	-
5	EDO	C	1904	-	-	1/1/1/1	-
5	EDO	C	1910	-	-	1/1/1/1	-
5	EDO	A	1906	-	-	1/1/1/1	-
5	EDO	C	1906	-	-	1/1/1/1	-
4	PNS	B	1901	1	-	1/24/26/27	-
5	EDO	B	1904	-	-	1/1/1/1	-
5	EDO	E	1907	-	-	1/1/1/1	-
5	EDO	E	1913	-	-	1/1/1/1	-
5	EDO	A	1903	-	-	1/1/1/1	-
5	EDO	D	1905	-	-	1/1/1/1	-
5	EDO	A	1907	-	-	1/1/1/1	-
4	PNS	E	1901	1	-	1/24/26/27	-
5	EDO	B	1911	-	-	1/1/1/1	-
5	EDO	D	1910	-	-	0/1/1/1	-
5	EDO	D	1903	-	-	1/1/1/1	-
5	EDO	F	1908	-	-	0/1/1/1	-
5	EDO	F	1903	-	-	0/1/1/1	-
5	EDO	B	1912	-	-	1/1/1/1	-
5	EDO	E	1910	-	-	0/1/1/1	-
5	EDO	E	1902	-	-	0/1/1/1	-
5	EDO	F	1902	-	-	0/1/1/1	-
5	EDO	J	2103	-	-	0/1/1/1	-
7	A2P	F	1912	-	-	9/11/31/31	0/3/3/3
5	EDO	D	1912	-	-	1/1/1/1	-
5	EDO	D	1911	-	-	1/1/1/1	-
5	EDO	B	1906	-	-	0/1/1/1	-
5	EDO	E	1905	-	-	1/1/1/1	-
5	EDO	D	1914	-	-	1/1/1/1	-
5	EDO	C	1908	-	-	1/1/1/1	-
7	A2P	C	1917	-	-	6/11/31/31	0/3/3/3
4	PNS	F	1901	1	-	3/24/26/27	-
5	EDO	F	1907	-	-	0/1/1/1	-
5	EDO	C	1912	-	-	1/1/1/1	-
5	EDO	B	1910	-	-	1/1/1/1	-
5	EDO	D	1904	-	-	1/1/1/1	-
5	EDO	J	2104	-	-	0/1/1/1	-
5	EDO	E	1912	-	-	0/1/1/1	-
5	EDO	A	1908	-	-	1/1/1/1	-
4	PNS	C	1901	1	-	1/24/26/27	-
4	PNS	A	1901	1	-	1/24/26/27	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	1905	-	-	1/1/1/1	-
5	EDO	F	1904	-	-	0/1/1/1	-
5	EDO	E	1904	-	-	0/1/1/1	-
5	EDO	E	1906	-	-	1/1/1/1	-
5	EDO	A	1910	-	-	1/1/1/1	-
5	EDO	D	1907	-	-	1/1/1/1	-
5	EDO	D	1902	-	-	1/1/1/1	-
10	FMN	G	2101	-	-	5/18/18/18	0/3/3/3
11	MLI	G	2102	-	-	0/0/4/4	-
5	EDO	H	2105	-	-	1/1/1/1	-
5	EDO	A	1902	-	-	1/1/1/1	-
5	EDO	E	1903	-	-	1/1/1/1	-
4	PNS	D	1901	1	-	0/24/26/27	-
5	EDO	D	1908	-	-	1/1/1/1	-
5	EDO	D	1909	-	-	1/1/1/1	-
5	EDO	C	1907	-	-	1/1/1/1	-
5	EDO	E	1911	-	-	1/1/1/1	-
11	MLI	J	2102	-	-	0/0/4/4	-
5	EDO	D	1906	-	-	1/1/1/1	-
5	EDO	A	1905	-	-	1/1/1/1	-
5	EDO	A	1909	-	-	0/1/1/1	-
5	EDO	F	1909	-	-	0/1/1/1	-
7	A2P	E	1917	-	-	6/11/31/31	0/3/3/3
10	FMN	I	2101	-	-	6/18/18/18	0/3/3/3
5	EDO	F	1906	-	-	1/1/1/1	-
7	A2P	B	1918	-	-	5/11/31/31	0/3/3/3

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	2101	FMN	C4A-C10	10.44	1.49	1.38
10	J	2101	FMN	C4A-C10	9.83	1.48	1.38
10	H	2101	FMN	C4A-C10	9.82	1.48	1.38
10	L	2101	FMN	C4A-C10	9.62	1.48	1.38
10	G	2101	FMN	C4A-C10	9.13	1.47	1.38

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	2101	FMN	C4-N3-C2	9.37	123.05	115.14
10	J	2101	FMN	C4-N3-C2	9.37	123.05	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	2101	FMN	C4-N3-C2	9.21	122.92	115.14
10	L	2101	FMN	C4-N3-C2	8.65	122.45	115.14
10	G	2101	FMN	C4-N3-C2	8.52	122.34	115.14

There are no chirality outliers.

5 of 114 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1918	A2P	C5'-O5'-P2-O4P
7	A	1918	A2P	C5'-O5'-P2-O6P
7	D	1923	A2P	C5'-O5'-P2-O5P
7	D	1923	A2P	C5'-O5'-P2-O6P
10	L	2101	FMN	C3'-C4'-C5'-O5'

There are no ring outliers.

25 monomers are involved in 64 short contacts:

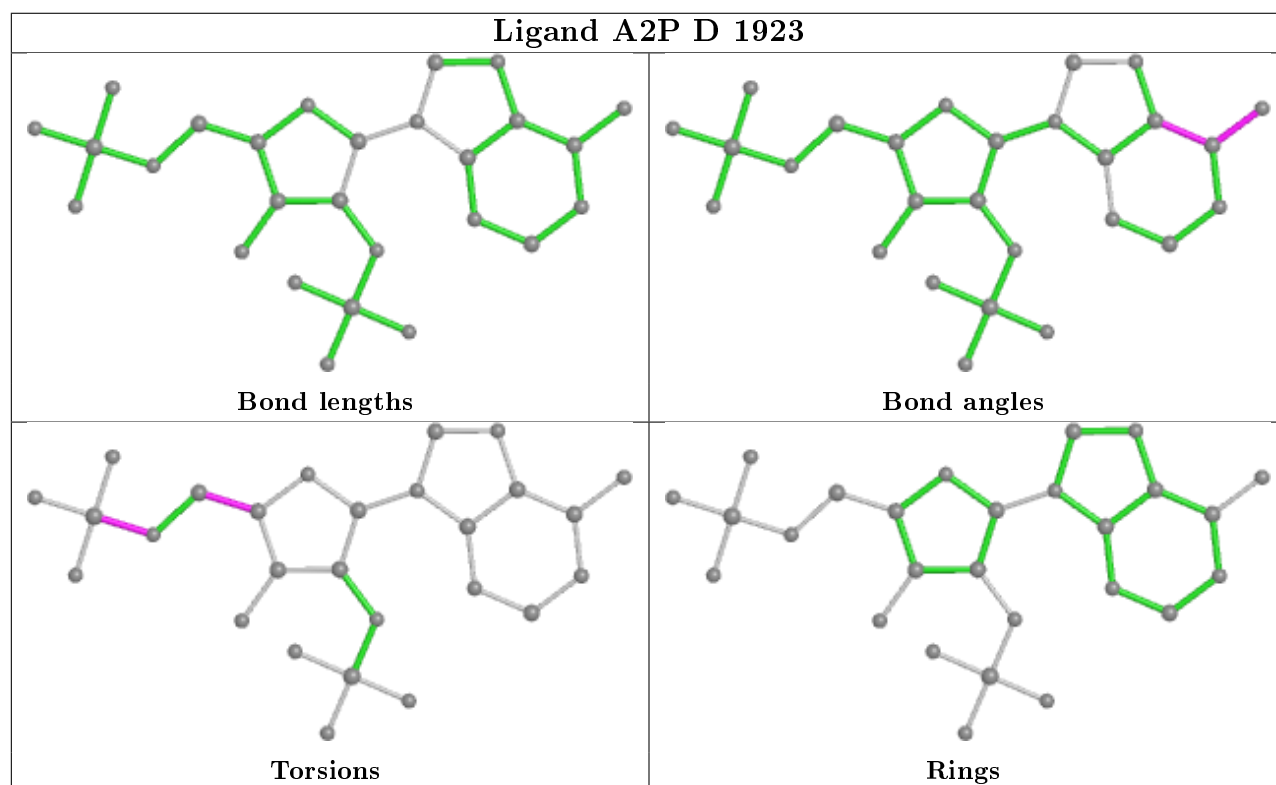
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1923	A2P	3	0
10	H	2101	FMN	4	0
8	B	1902	ACT	1	0
10	J	2101	FMN	7	0
7	A	1918	A2P	3	0
10	L	2101	FMN	5	0
10	K	2101	FMN	5	0
5	J	2105	EDO	1	0
4	B	1901	PNS	1	0
8	C	1903	ACT	2	0
5	D	1910	EDO	1	0
7	F	1912	A2P	1	0
5	B	1906	EDO	3	0
7	C	1917	A2P	2	0
4	F	1901	PNS	2	0
5	B	1910	EDO	1	0
5	J	2104	EDO	1	0
4	A	1901	PNS	1	0
10	G	2101	FMN	4	0
11	G	2102	MLI	1	0
5	C	1907	EDO	1	0
11	J	2102	MLI	2	0
7	E	1917	A2P	2	0

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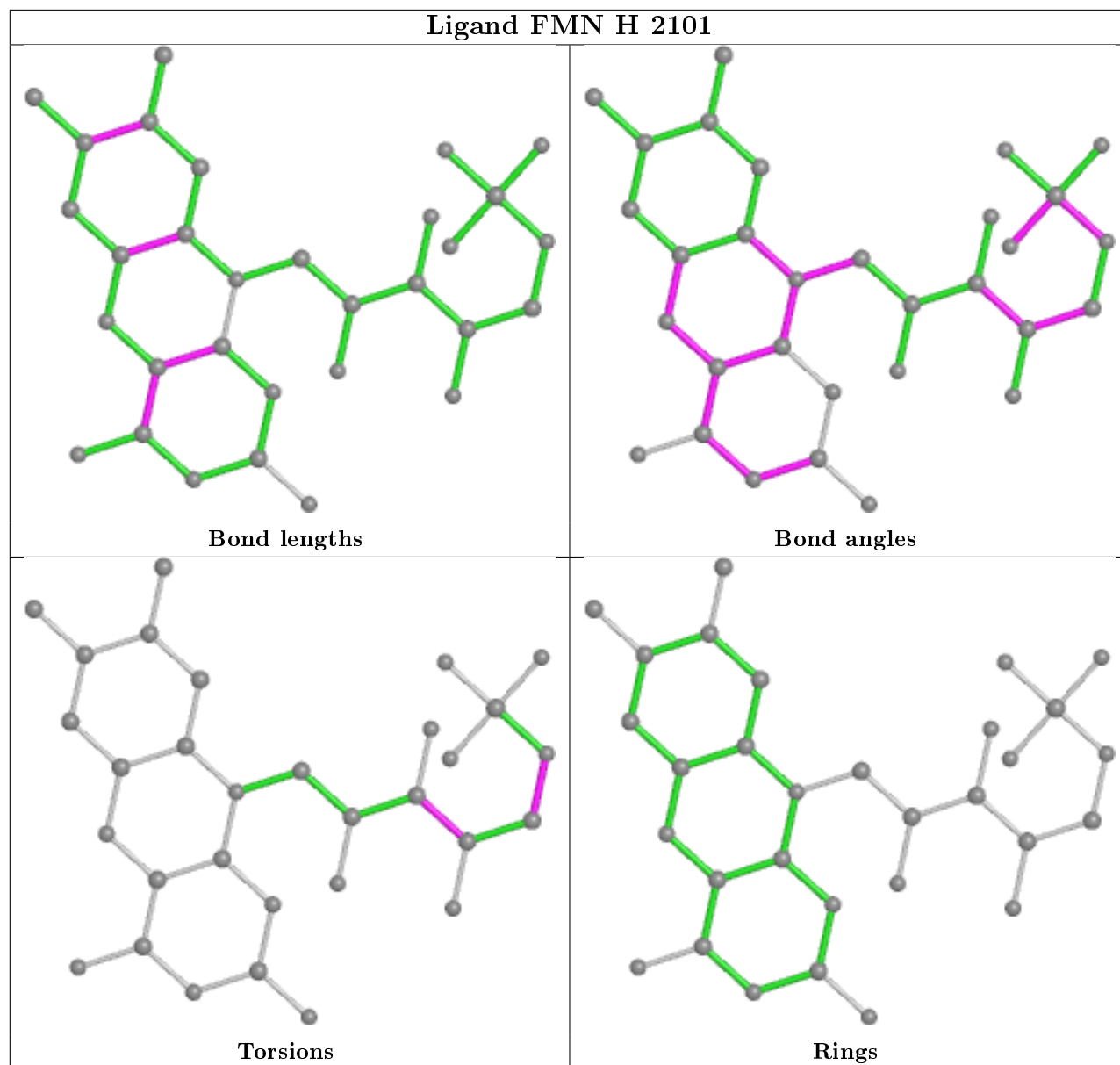
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	2101	FMN	5	0
7	B	1918	A2P	5	0

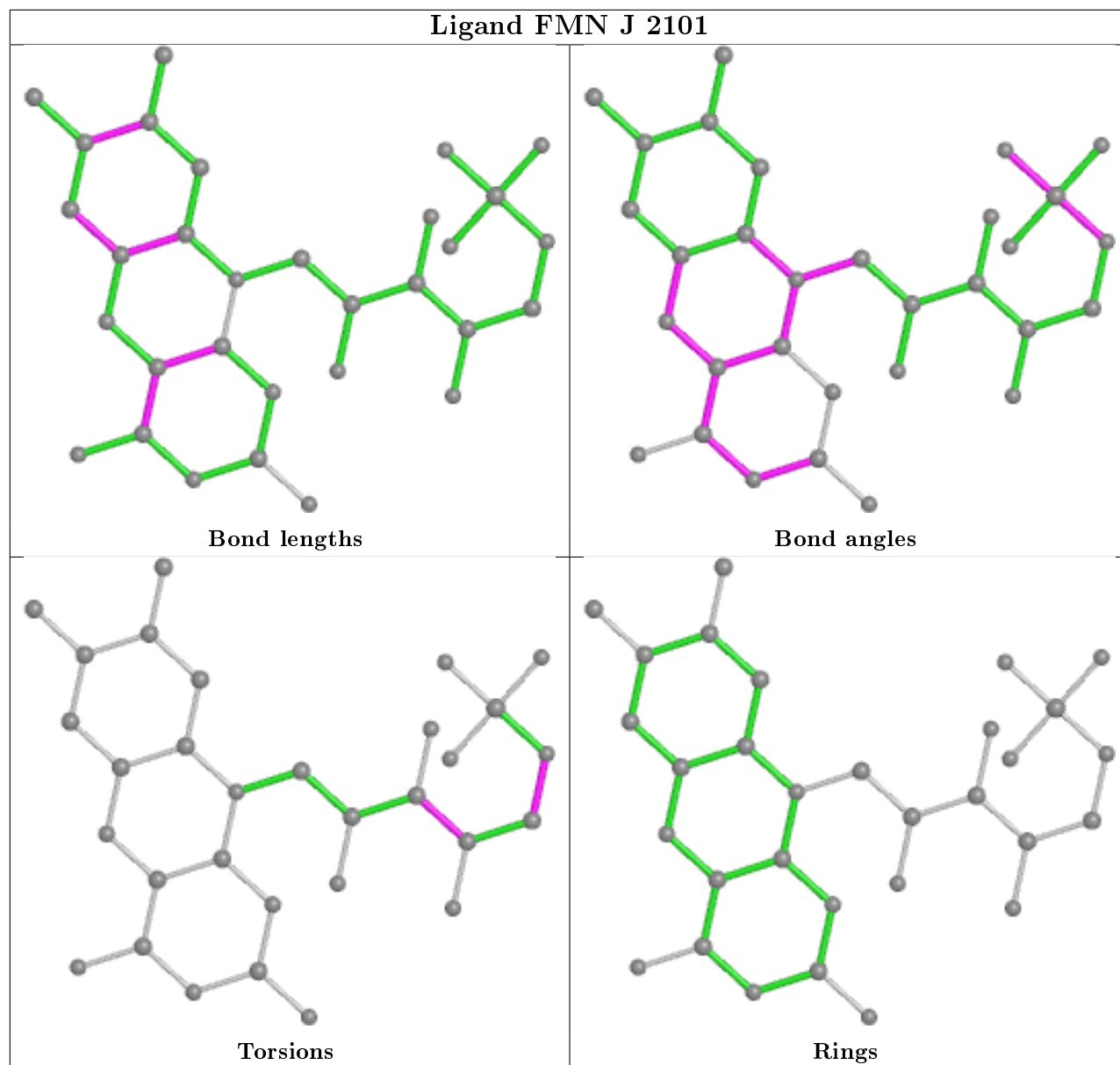
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

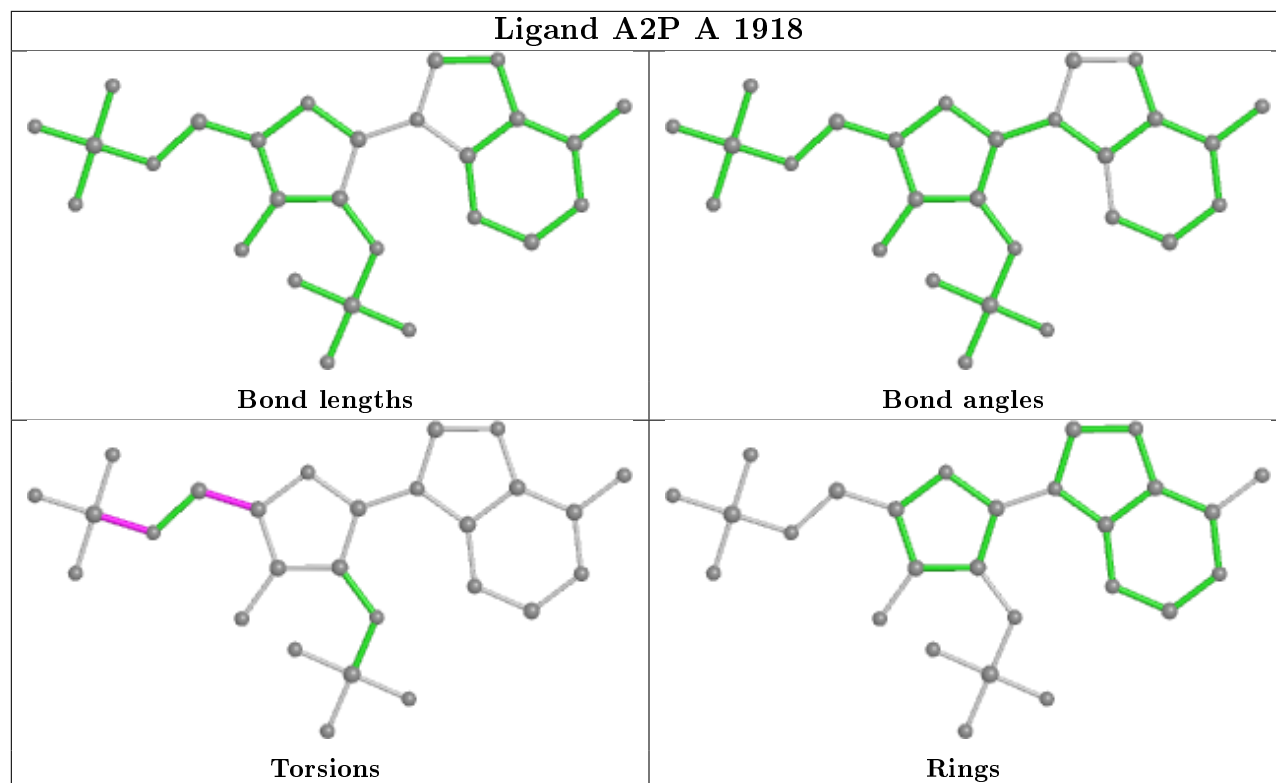


## Ligand FMN H 2101

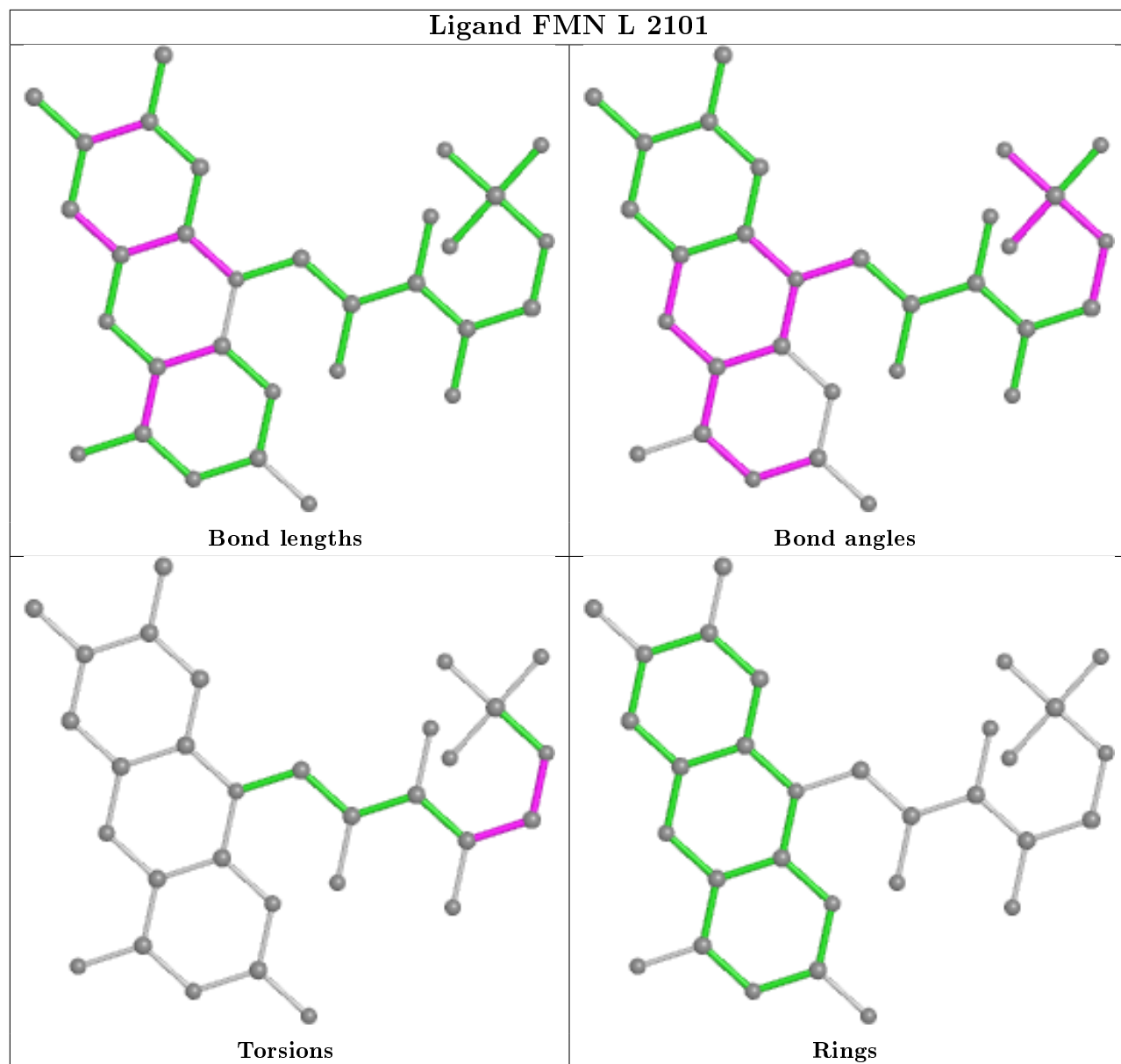


## Ligand FMN J 2101



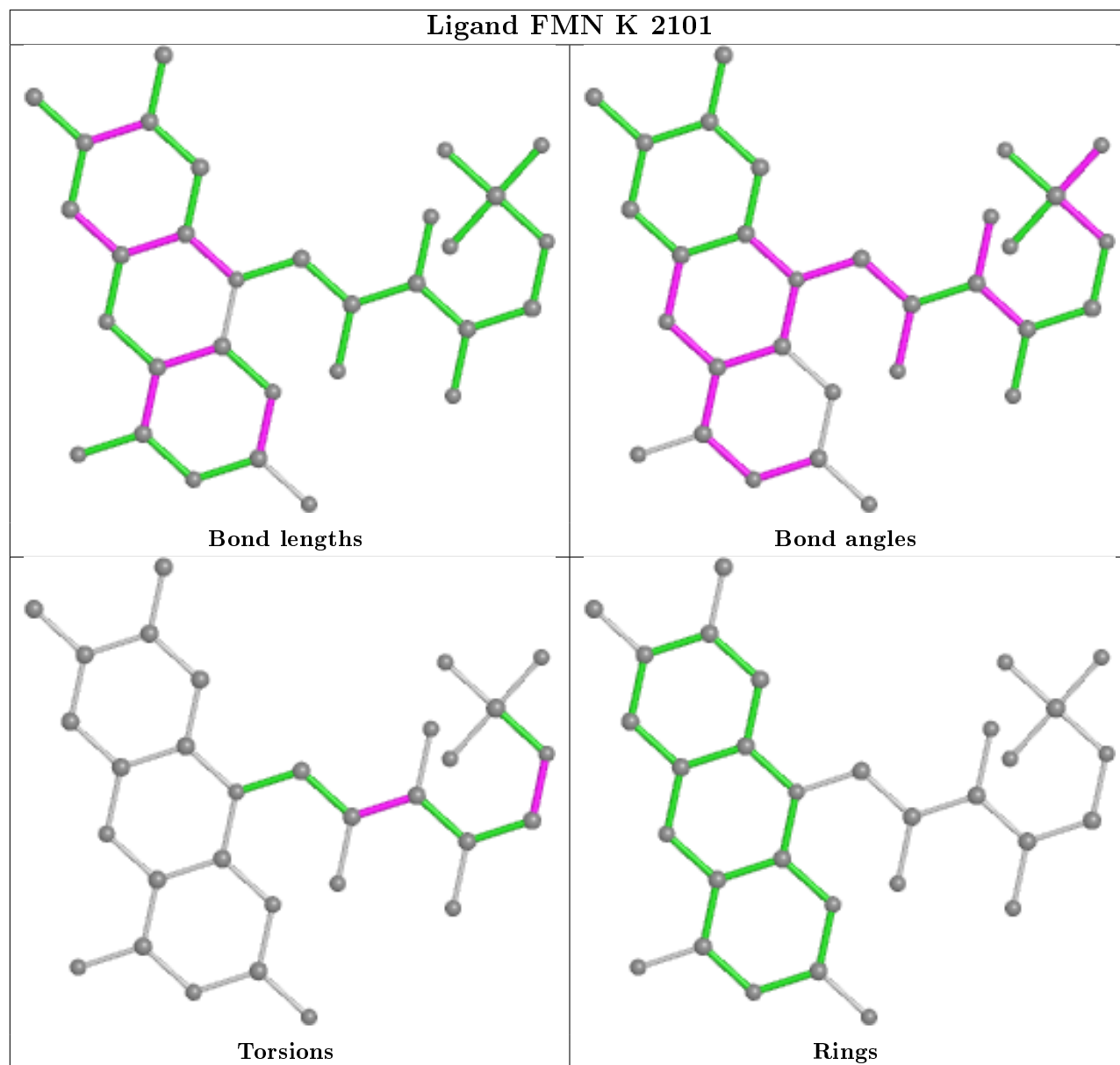


## Ligand FMN L 2101

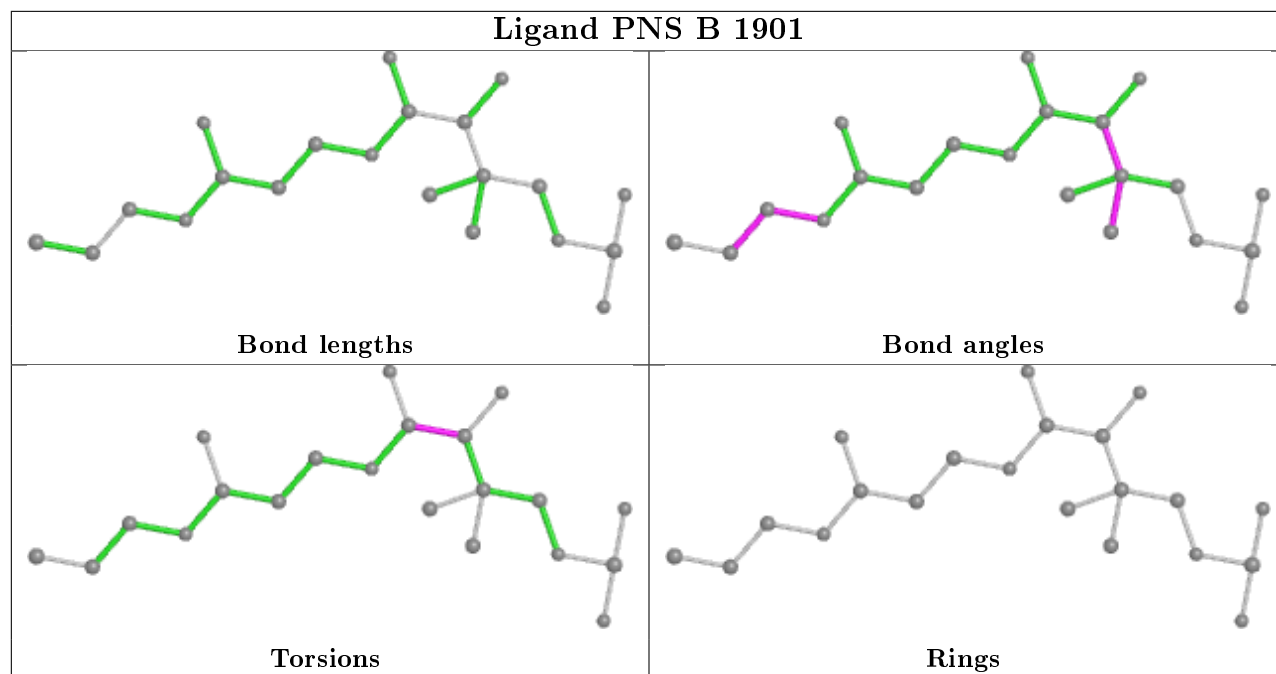




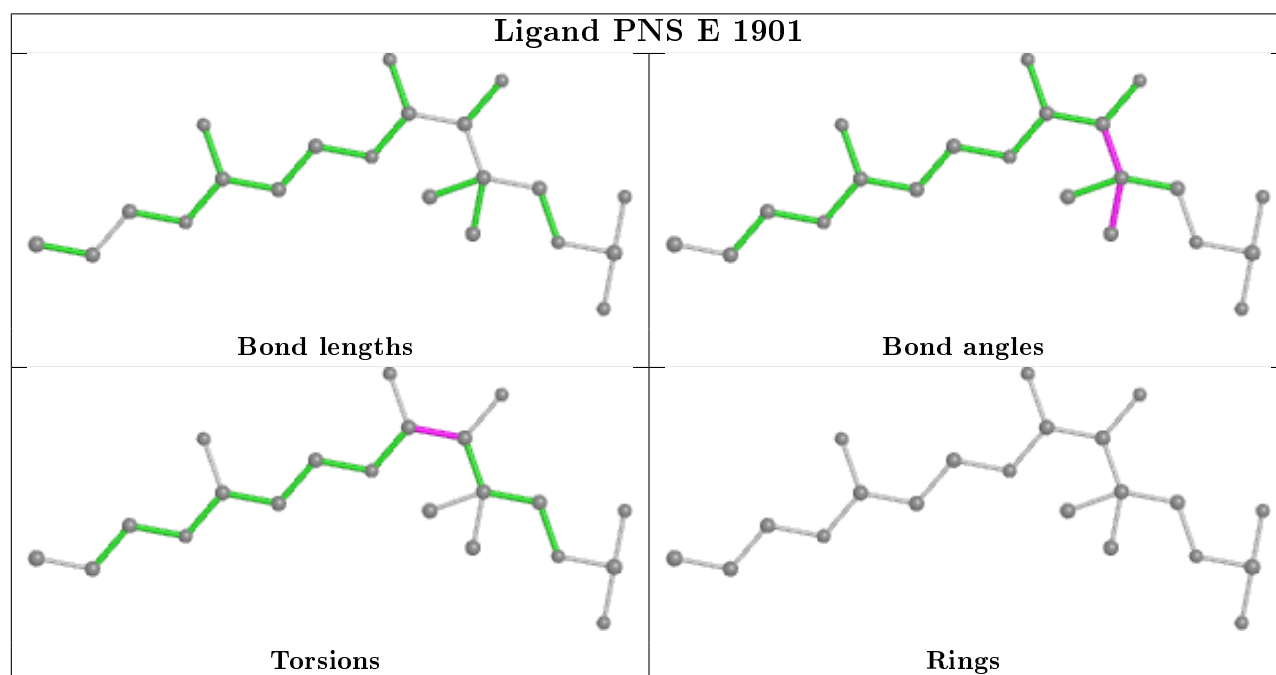
## Ligand FMN K 2101

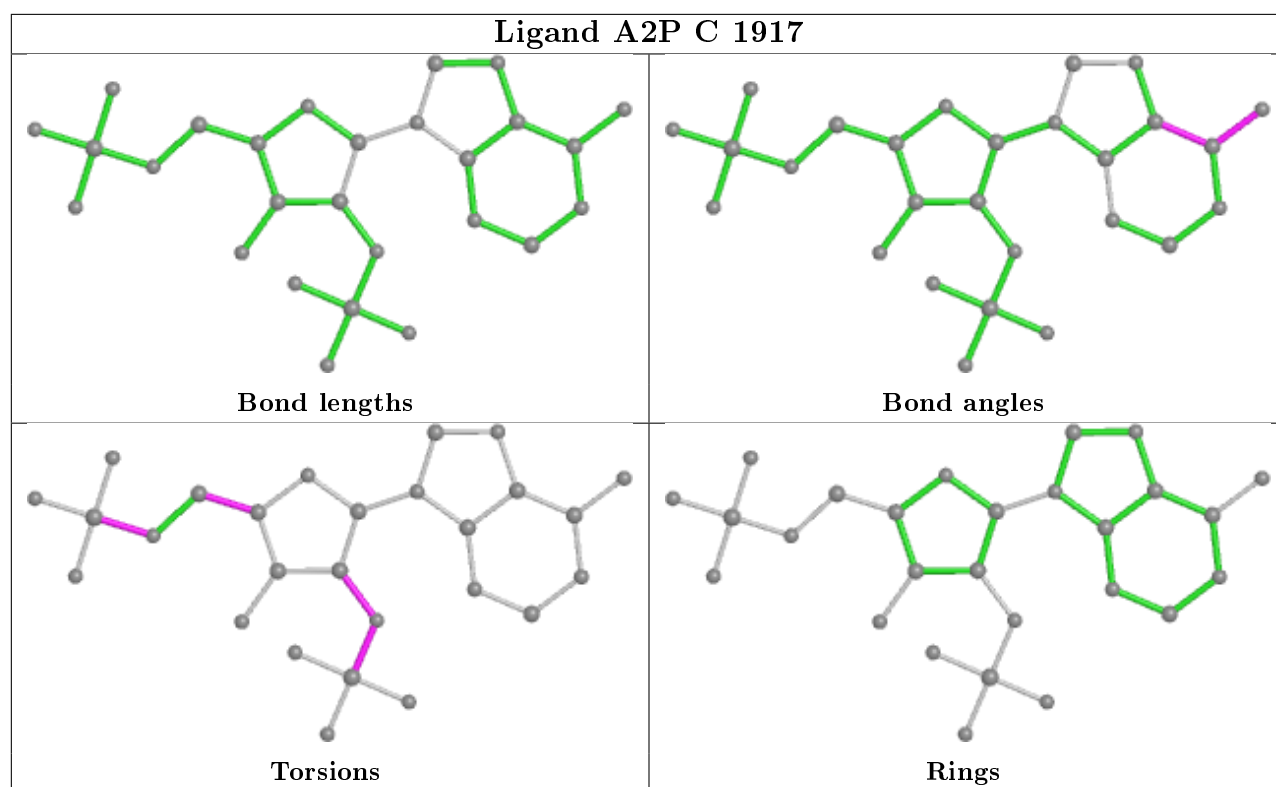
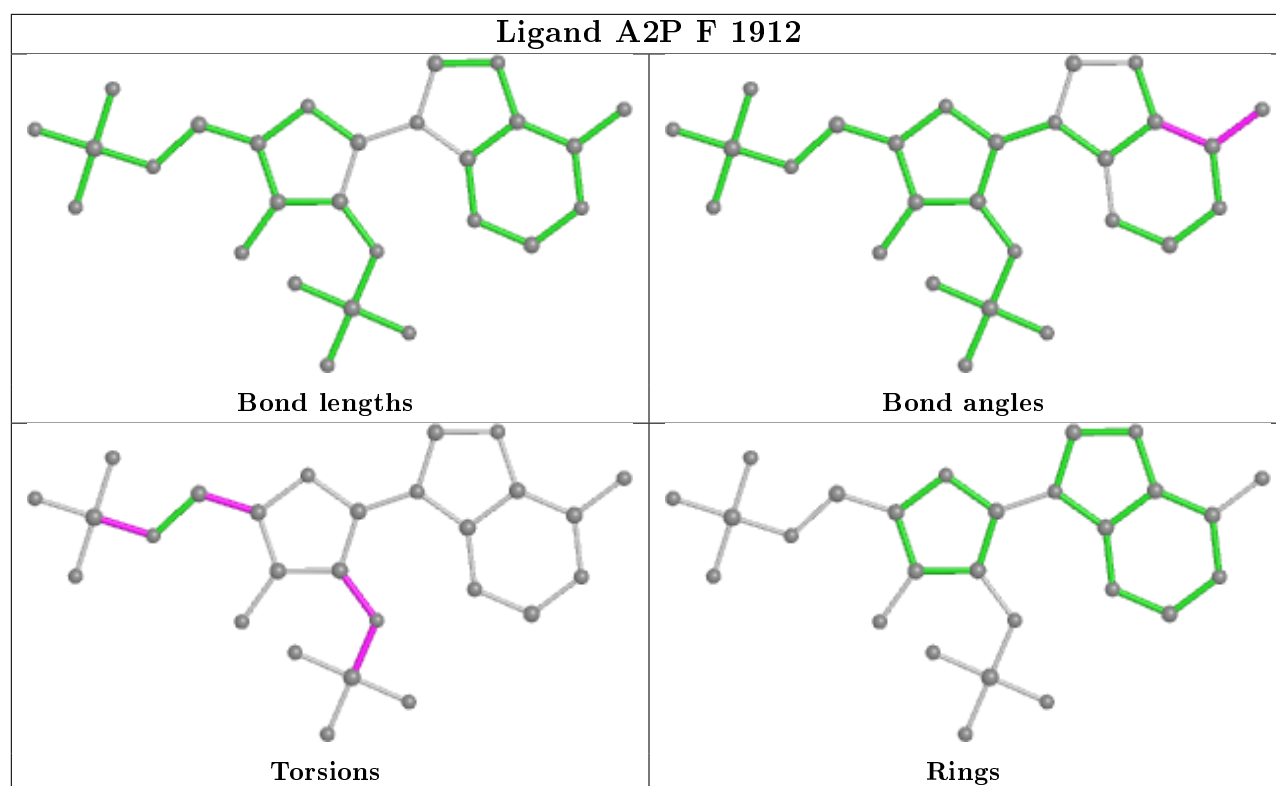


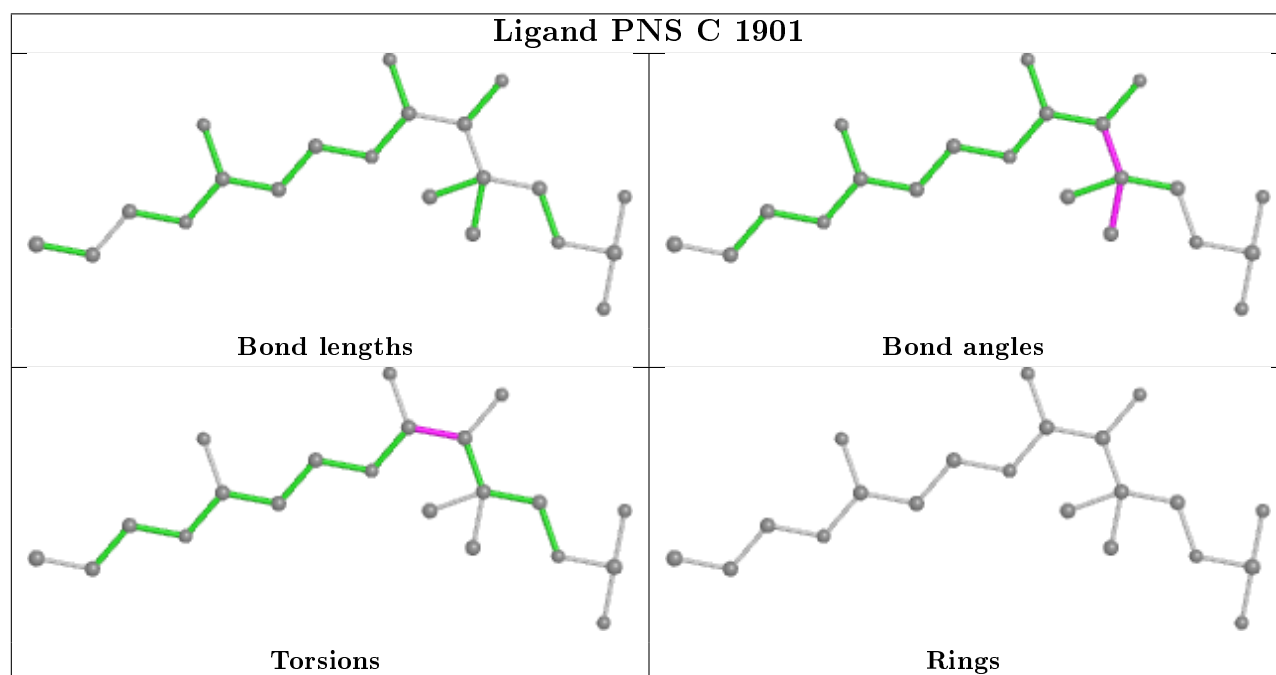
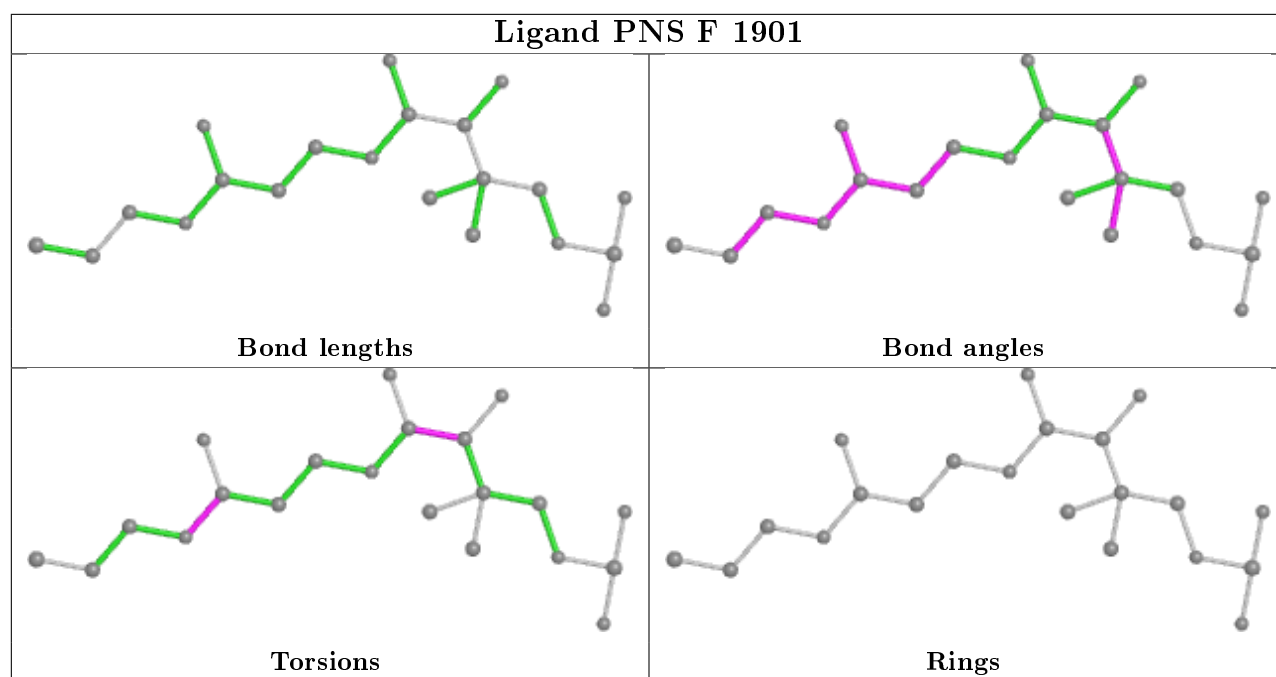
## Ligand PNS B 1901

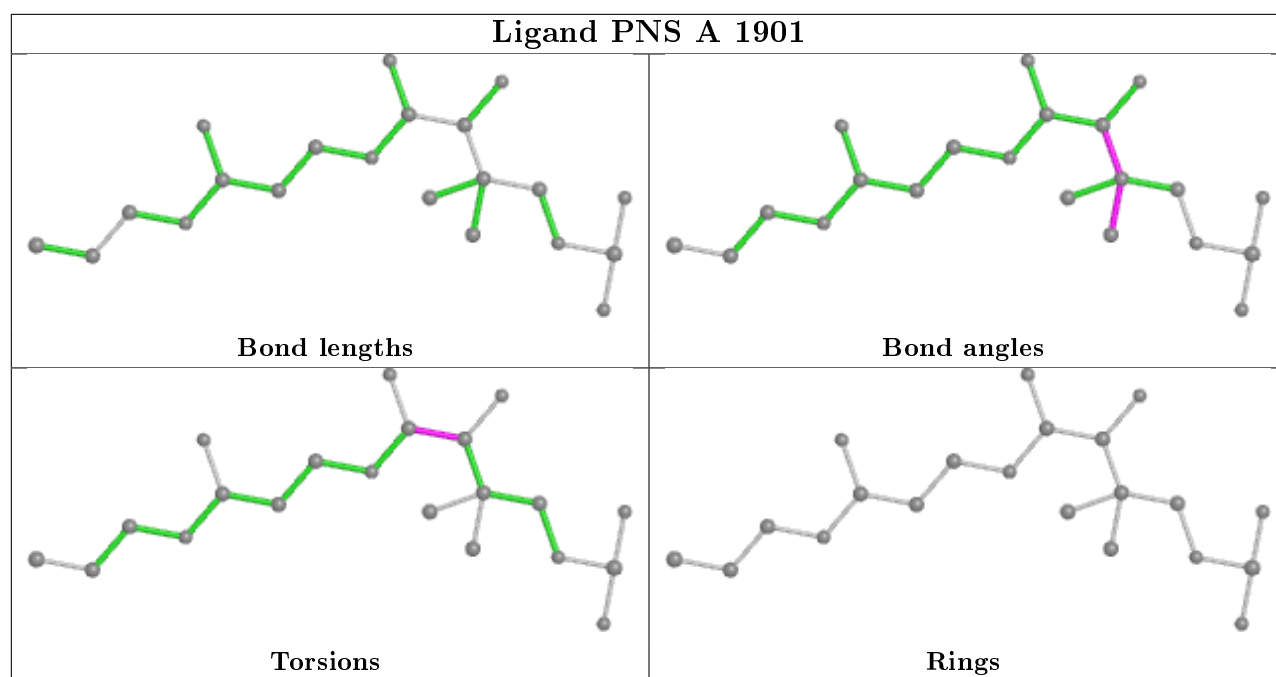


## Ligand PNS E 1901

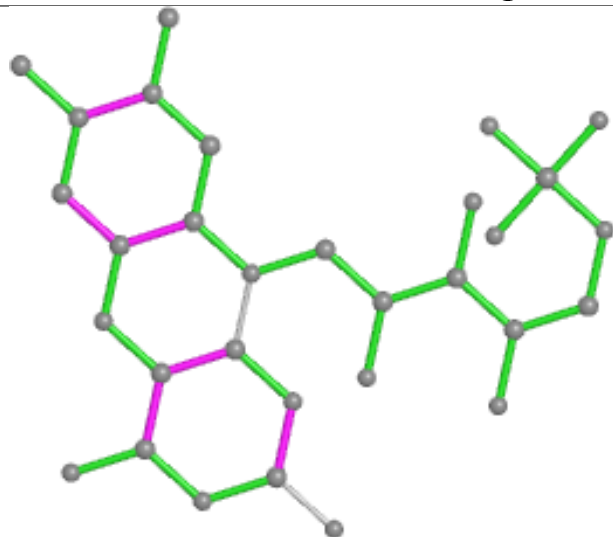




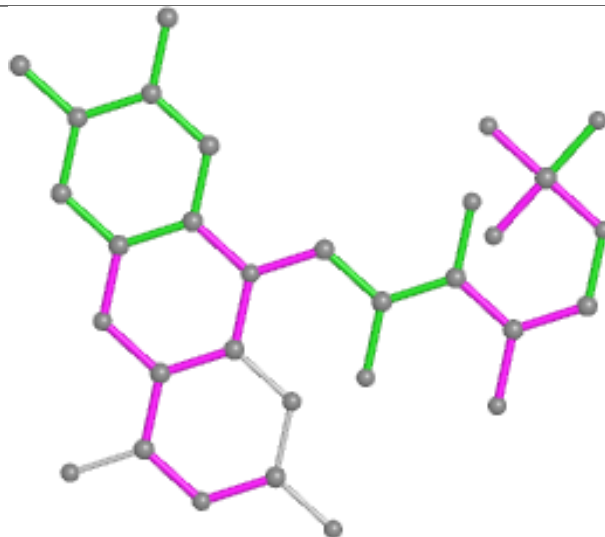




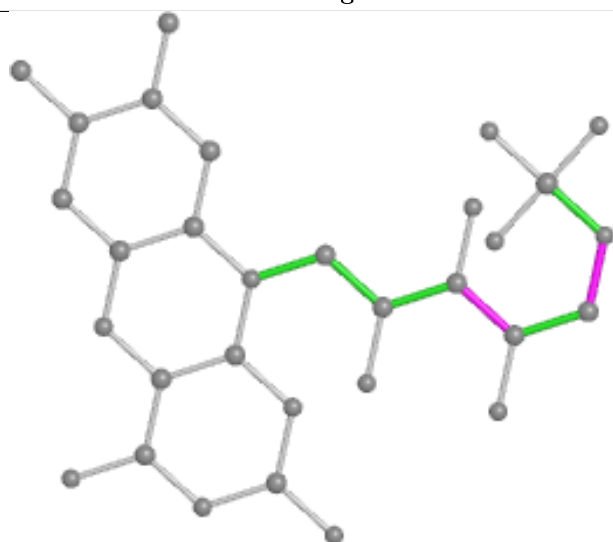
## Ligand FMN G 2101



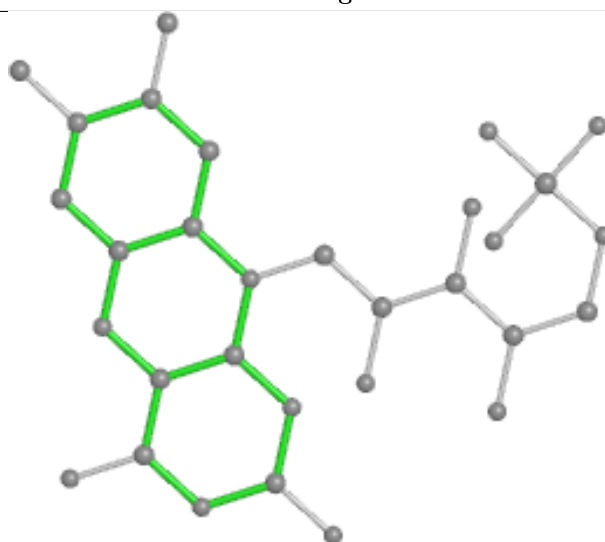
Bond lengths



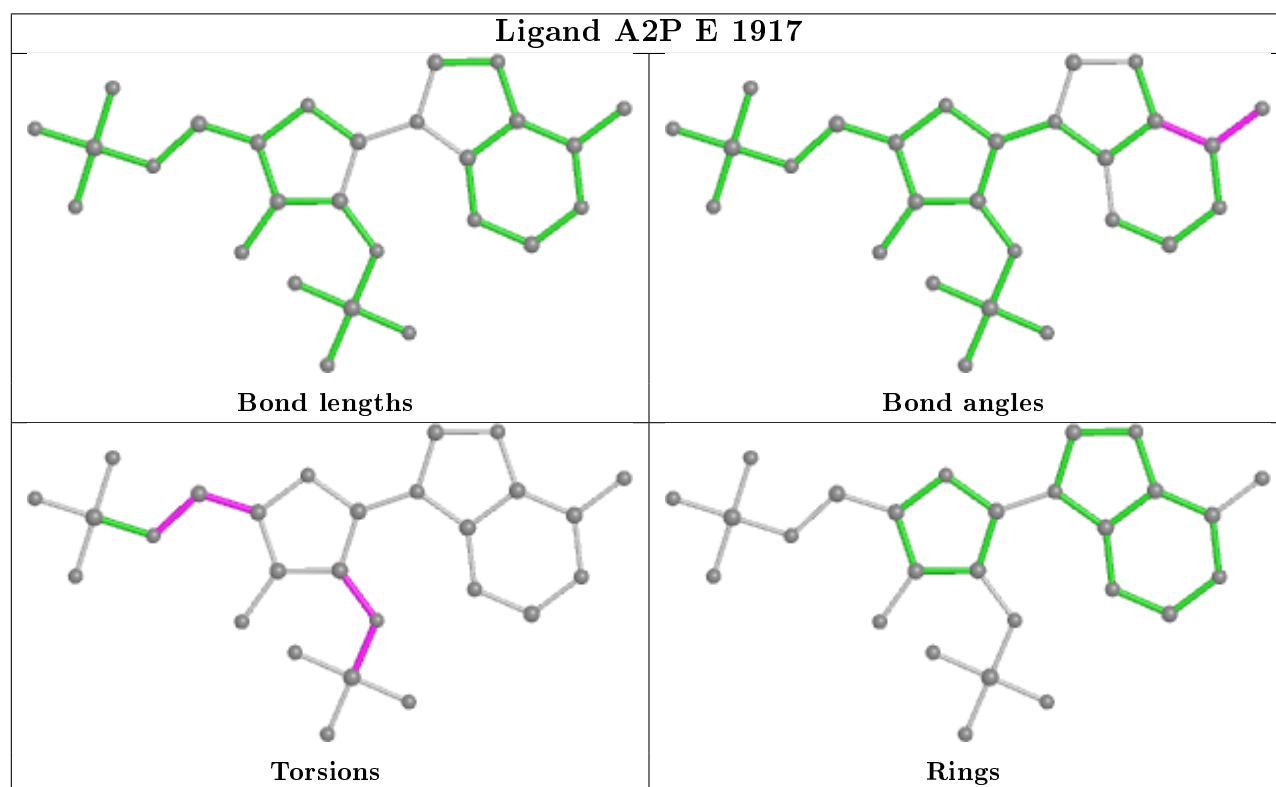
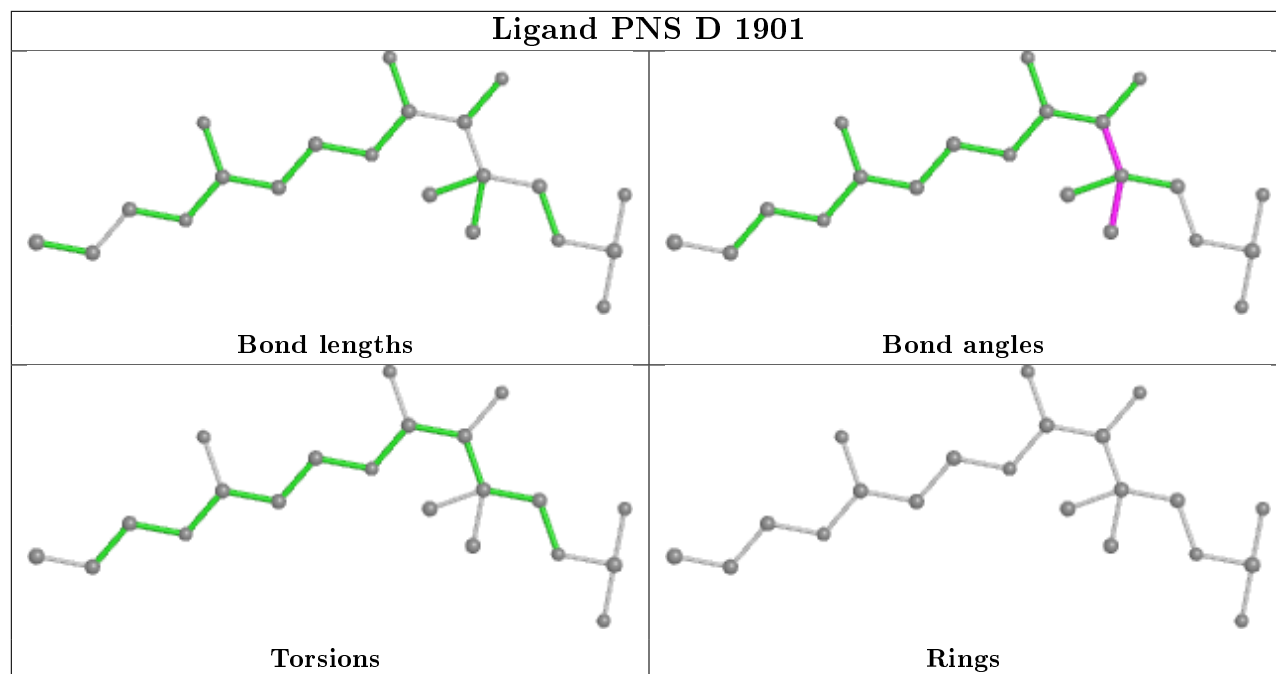
Bond angles

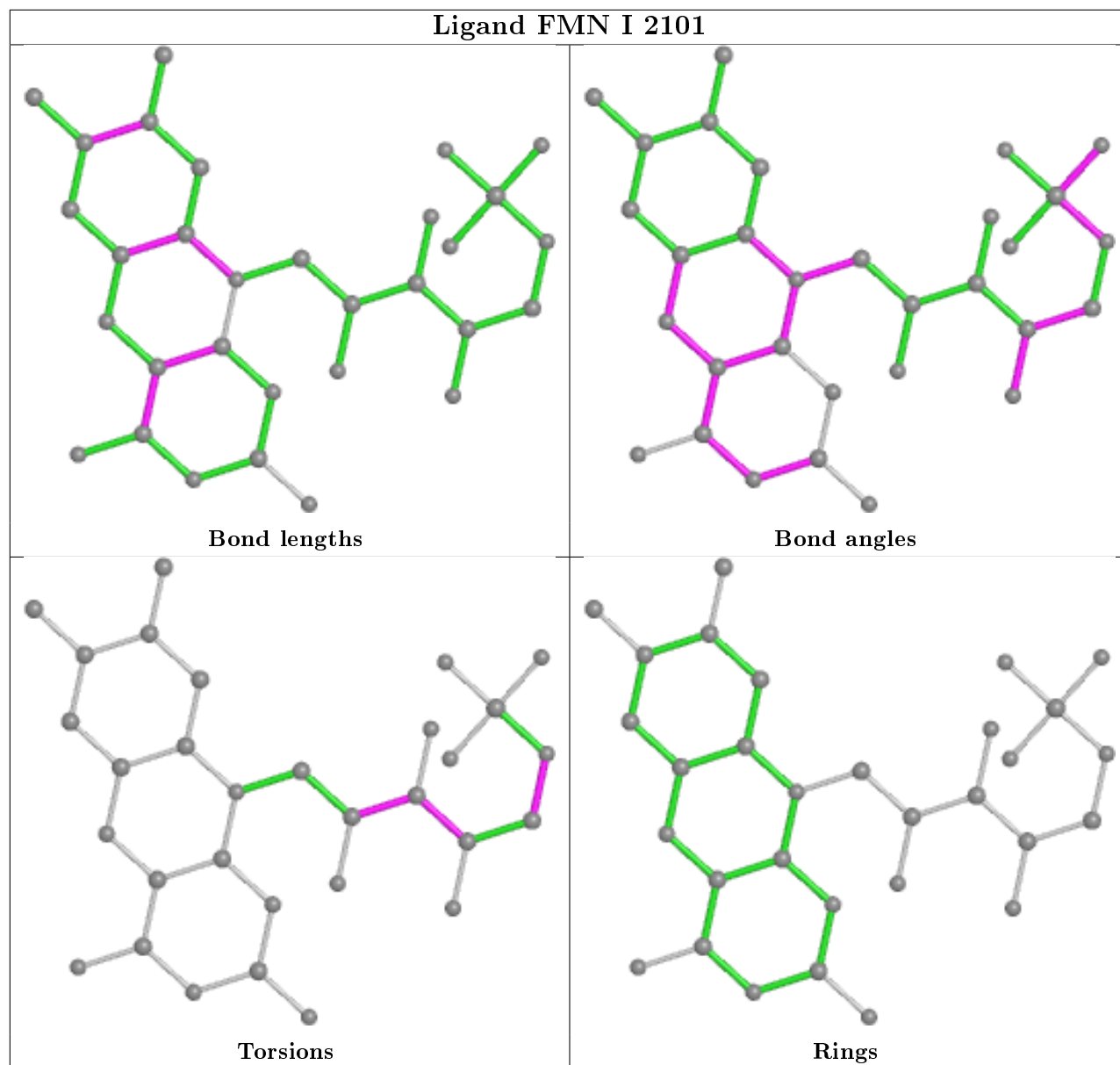


Torsions

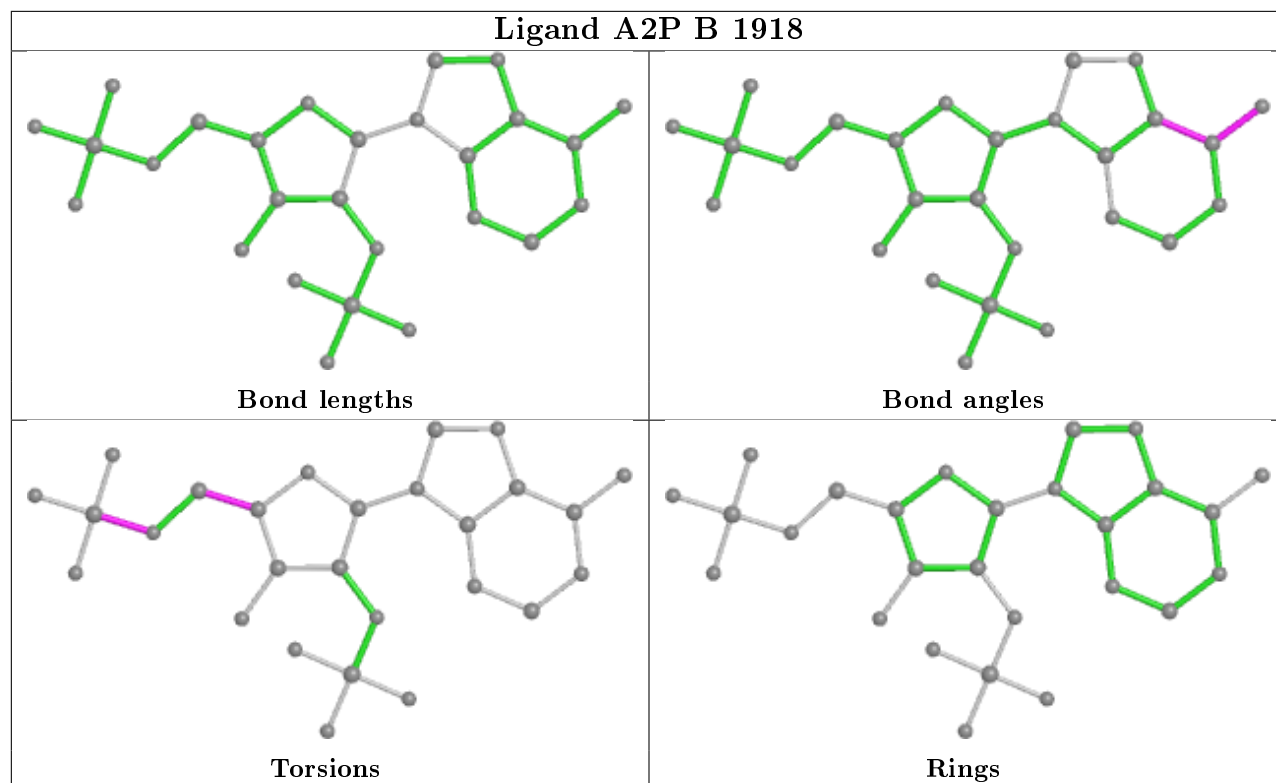


Rings









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1760/1887 (93%)	0.23	32 (1%) 68 61	32, 54, 115, 158	0
1	B	1759/1887 (93%)	0.23	25 (1%) 75 69	29, 53, 108, 154	0
1	C	1759/1887 (93%)	0.19	25 (1%) 75 69	31, 53, 112, 166	0
1	D	1765/1887 (93%)	0.21	12 (0%) 87 84	27, 47, 111, 154	0
1	E	1759/1887 (93%)	0.20	26 (1%) 73 67	35, 57, 109, 162	0
1	F	1759/1887 (93%)	0.19	21 (1%) 79 73	34, 59, 117, 172	0
2	G	2036/2051 (99%)	0.18	38 (1%) 66 59	42, 70, 130, 175	0
2	J	2035/2051 (99%)	0.22	38 (1%) 66 59	37, 69, 135, 189	0
3	H	2034/2051 (99%)	0.15	12 (0%) 89 86	39, 67, 119, 162	0
3	I	2033/2051 (99%)	0.17	18 (0%) 84 80	48, 79, 124, 167	0
3	K	2034/2051 (99%)	0.23	32 (1%) 72 65	57, 87, 129, 175	0
3	L	2035/2051 (99%)	0.27	44 (2%) 62 52	56, 84, 137, 191	0
All	All	22768/23628 (96%)	0.21	323 (1%) 75 69	27, 71, 122, 191	0

The worst 5 of 323 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1830	GLY	10.0
1	E	599	MET	8.9
1	B	1831	GLY	8.7
1	F	1830	GLY	8.3
1	A	1829	GLY	8.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	J8W	I	1808	12/13	0.88	0.23	79,93,103,106	0
3	J8W	L	1808	12/13	0.88	0.23	97,105,108,110	0
3	J8W	K	1808	12/13	0.91	0.21	83,92,98,98	0
3	J8W	H	1808	12/13	0.94	0.22	66,82,88,89	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	E	1908	4/4	0.61	0.28	76,79,81,82	0
5	EDO	F	1904	4/4	0.64	0.27	68,73,77,78	0
7	A2P	B	1918	27/27	0.68	0.43	87,126,138,145	0
5	EDO	F	1902	4/4	0.72	0.39	75,80,85,89	0
8	ACT	B	1902	4/4	0.73	0.41	68,72,75,76	0
5	EDO	J	2104	4/4	0.74	0.22	68,70,71,71	0
6	NA	J	2108	1/1	0.74	0.13	60,60,60,60	0
8	ACT	H	2102	4/4	0.74	0.31	80,82,86,89	0
5	EDO	C	1910	4/4	0.74	0.30	79,83,84,86	0
7	A2P	F	1912	27/27	0.77	0.43	86,121,152,158	0
7	A2P	A	1918	27/27	0.77	0.48	87,121,166,169	0
5	EDO	E	1912	4/4	0.77	0.37	91,93,93,97	0
6	NA	C	1914	1/1	0.77	0.52	60,60,60,60	0
9	PGE	E	1918	10/10	0.77	0.39	88,99,106,107	0
5	EDO	C	1908	4/4	0.77	0.27	60,69,73,74	0
5	EDO	D	1912	4/4	0.79	0.27	79,81,81,82	0
5	EDO	C	1907	4/4	0.79	0.32	75,78,80,81	0
5	EDO	A	1909	4/4	0.79	0.38	64,64,71,71	0
7	A2P	D	1923	27/27	0.79	0.35	74,107,137,145	0
5	EDO	D	1906	4/4	0.80	0.24	51,52,58,59	0
6	NA	G	2104	1/1	0.80	0.18	59,59,59,59	0
7	A2P	E	1917	27/27	0.80	0.45	83,114,130,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	F	1906	4/4	0.80	0.27	71,74,76,77	0
5	EDO	J	2105	4/4	0.80	0.33	73,77,78,79	0
8	ACT	C	1903	4/4	0.82	0.49	59,69,73,75	0
8	ACT	H	2104	4/4	0.82	0.29	81,84,84,85	0
6	NA	E	1915	1/1	0.82	0.09	50,50,50,50	0
6	NA	I	2102	1/1	0.83	0.17	84,84,84,84	0
5	EDO	A	1907	4/4	0.83	0.39	69,71,74,75	0
5	EDO	C	1911	4/4	0.83	0.40	64,65,71,71	0
5	EDO	B	1903	4/4	0.83	0.17	70,76,77,79	0
8	ACT	H	2103	4/4	0.84	0.31	66,66,70,73	0
6	NA	D	1918	1/1	0.84	0.34	56,56,56,56	0
6	NA	B	1915	1/1	0.84	0.13	49,49,49,49	0
5	EDO	C	1909	4/4	0.84	0.28	72,78,79,80	0
7	A2P	C	1917	27/27	0.84	0.34	66,97,150,153	0
6	NA	H	2107	1/1	0.85	0.12	49,49,49,49	0
6	NA	F	1910	1/1	0.85	0.67	65,65,65,65	0
5	EDO	F	1905	4/4	0.85	0.36	65,67,67,67	0
5	EDO	H	2105	4/4	0.86	0.20	68,72,74,76	0
5	EDO	F	1909	4/4	0.86	0.29	54,54,56,56	0
5	EDO	B	1910	4/4	0.86	0.25	69,72,76,78	0
5	EDO	A	1908	4/4	0.86	0.21	59,60,60,60	0
5	EDO	B	1911	4/4	0.86	0.36	55,57,58,59	0
6	NA	D	1920	1/1	0.87	0.26	45,45,45,45	0
5	EDO	A	1911	4/4	0.87	0.25	83,84,90,91	0
5	EDO	B	1912	4/4	0.87	0.21	74,78,78,80	0
5	EDO	A	1903	4/4	0.87	0.22	56,60,60,61	0
6	NA	A	1916	1/1	0.87	0.47	51,51,51,51	0
5	EDO	E	1910	4/4	0.88	0.32	80,82,84,85	0
5	EDO	A	1905	4/4	0.88	0.17	57,60,60,61	0
5	EDO	C	1906	4/4	0.88	0.21	67,68,72,74	0
5	EDO	D	1902	4/4	0.89	0.30	58,59,59,60	0
5	EDO	D	1911	4/4	0.89	0.18	60,61,61,62	0
5	EDO	B	1906	4/4	0.89	0.32	52,54,58,65	0
5	EDO	E	1911	4/4	0.89	0.25	69,69,72,72	0
6	NA	C	1916	1/1	0.89	0.70	61,61,61,61	0
5	EDO	D	1903	4/4	0.89	0.21	46,52,55,56	0
5	EDO	B	1907	4/4	0.90	0.36	57,58,58,59	0
5	EDO	J	2106	4/4	0.90	0.33	72,72,73,73	0
5	EDO	A	1910	4/4	0.90	0.32	64,69,70,70	0
5	EDO	E	1905	4/4	0.90	0.41	64,68,70,72	0
6	NA	A	1915	1/1	0.90	0.09	51,51,51,51	0
5	EDO	D	1907	4/4	0.90	0.25	56,63,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	E	1909	4/4	0.91	0.22	69,70,71,72	0
5	EDO	D	1913	4/4	0.91	0.14	61,61,63,66	0
6	NA	F	1911	1/1	0.91	0.14	62,62,62,62	0
6	NA	A	1913	1/1	0.91	0.38	42,42,42,42	0
5	EDO	C	1904	4/4	0.91	0.46	74,76,78,79	0
5	EDO	D	1909	4/4	0.91	0.27	60,61,62,63	0
5	EDO	E	1906	4/4	0.91	0.14	68,75,75,75	0
6	NA	D	1916	1/1	0.91	0.10	55,55,55,55	0
6	NA	K	2103	1/1	0.92	0.16	69,69,69,69	0
5	EDO	C	1905	4/4	0.92	0.34	54,57,61,62	0
5	EDO	B	1909	4/4	0.92	0.22	50,53,54,55	0
5	EDO	C	1912	4/4	0.92	0.41	50,52,53,54	0
6	NA	G	2103	1/1	0.92	0.12	37,37,37,37	0
6	NA	B	1917	1/1	0.92	0.44	47,47,47,47	0
6	NA	J	2107	1/1	0.92	0.17	38,38,38,38	0
11	MLI	J	2102	7/7	0.92	0.25	83,86,87,96	0
6	NA	A	1912	1/1	0.93	0.14	65,65,65,65	0
6	NA	E	1914	1/1	0.93	0.16	62,62,62,62	0
5	EDO	F	1908	4/4	0.93	0.45	83,88,92,93	0
6	NA	C	1915	1/1	0.93	0.74	62,62,62,62	0
4	PNS	B	1901	21/22	0.93	0.33	91,95,106,107	0
5	EDO	D	1914	4/4	0.93	0.29	49,52,54,56	0
10	FMN	K	2101	31/31	0.93	0.20	64,75,80,88	0
5	EDO	D	1904	4/4	0.93	0.22	58,63,66,68	0
5	EDO	E	1907	4/4	0.93	0.18	69,72,73,74	0
5	EDO	B	1908	4/4	0.94	0.17	58,62,62,62	0
5	EDO	E	1913	4/4	0.94	0.54	78,81,86,86	0
11	MLI	G	2102	7/7	0.94	0.27	78,86,91,92	0
5	EDO	E	1904	4/4	0.94	0.30	67,70,72,74	0
5	EDO	A	1904	4/4	0.94	0.37	59,63,65,65	0
4	PNS	F	1901	21/22	0.94	0.29	89,92,102,103	0
5	EDO	J	2103	4/4	0.94	0.22	69,71,71,71	0
4	PNS	C	1901	21/22	0.94	0.25	75,78,88,89	0
6	NA	A	1914	1/1	0.94	0.36	55,55,55,55	0
5	EDO	A	1906	4/4	0.95	0.30	53,58,58,59	0
6	NA	C	1913	1/1	0.95	0.07	56,56,56,56	0
6	NA	D	1921	1/1	0.95	0.15	52,52,52,52	0
5	EDO	D	1905	4/4	0.95	0.24	45,46,47,49	0
8	ACT	C	1902	4/4	0.95	0.24	59,62,63,65	0
4	PNS	E	1901	21/22	0.95	0.29	86,88,91,92	0
5	EDO	E	1902	4/4	0.95	0.40	51,51,51,52	0
6	NA	L	2103	1/1	0.95	0.17	66,66,66,66	0

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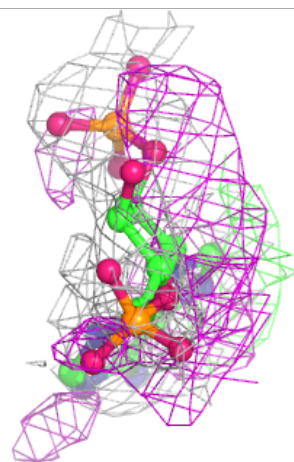
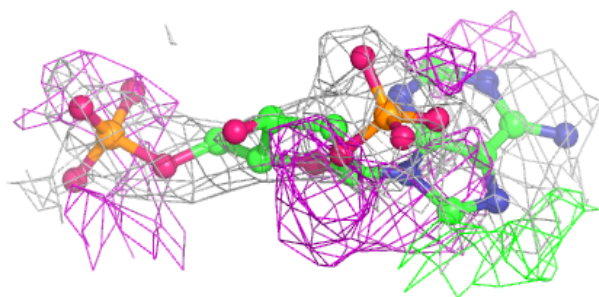
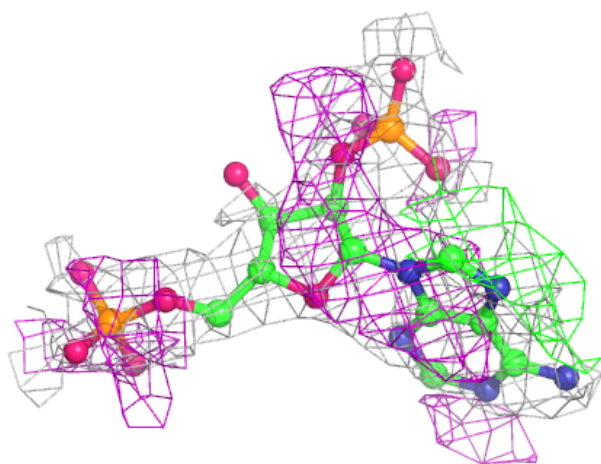
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NA	L	2102	1/1	0.95	0.10	46,46,46,46	0
5	EDO	B	1905	4/4	0.95	0.32	65,66,67,67	0
5	EDO	D	1910	4/4	0.95	0.23	59,63,64,64	0
5	EDO	B	1904	4/4	0.95	0.24	51,53,56,62	0
10	FMN	I	2101	31/31	0.95	0.21	66,73,78,79	0
4	PNS	D	1901	21/22	0.95	0.35	90,93,101,103	0
5	EDO	D	1908	4/4	0.95	0.30	54,56,58,58	0
6	NA	B	1914	1/1	0.96	0.15	43,43,43,43	0
6	NA	E	1916	1/1	0.96	0.23	51,51,51,51	0
4	PNS	A	1901	21/22	0.96	0.27	86,90,101,101	0
6	NA	A	1917	1/1	0.96	0.34	53,53,53,53	0
10	FMN	L	2101	31/31	0.96	0.20	54,62,68,81	0
6	NA	D	1922	1/1	0.96	0.54	46,46,46,46	0
5	EDO	A	1902	4/4	0.96	0.18	47,51,54,54	0
6	NA	B	1916	1/1	0.96	0.31	52,52,52,52	0
5	EDO	E	1903	4/4	0.97	0.24	50,54,55,56	0
6	NA	D	1915	1/1	0.97	0.11	49,49,49,49	0
10	FMN	J	2101	31/31	0.97	0.19	43,46,50,55	0
6	NA	K	2102	1/1	0.97	0.11	53,53,53,53	0
10	FMN	G	2101	31/31	0.97	0.21	46,49,53,56	0
5	EDO	F	1907	4/4	0.97	0.43	54,58,61,63	0
10	FMN	H	2101	31/31	0.97	0.21	43,50,54,61	0
6	NA	D	1917	1/1	0.97	0.46	46,46,46,46	0
5	EDO	F	1903	4/4	0.97	0.23	65,66,70,70	0
6	NA	H	2106	1/1	0.98	0.13	34,34,34,34	0
6	NA	D	1919	1/1	0.98	0.65	46,46,46,46	0
6	NA	B	1913	1/1	0.98	0.12	43,43,43,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

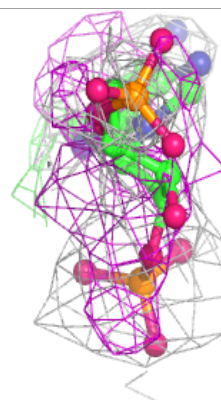
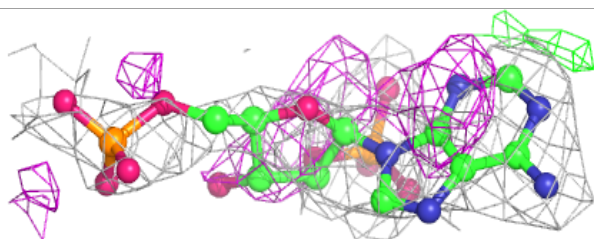
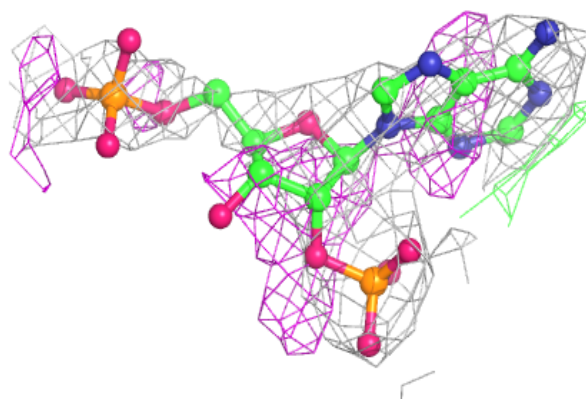
**Electron density around A2P B 1918:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

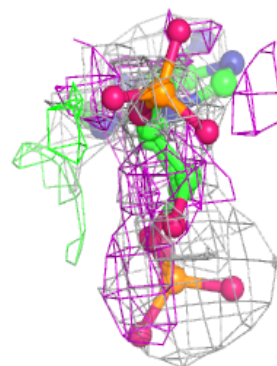
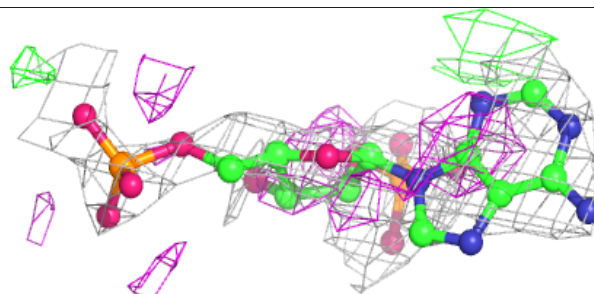
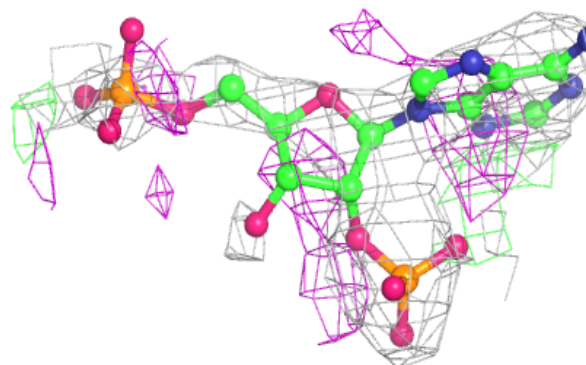


**Electron density around A2P F 1912:**

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and green (positive)

**Electron density around A2P A 1918:**

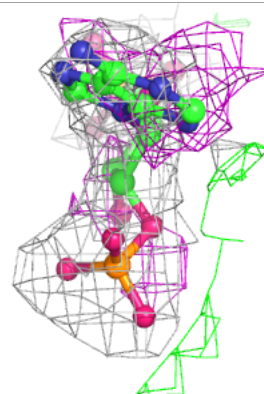
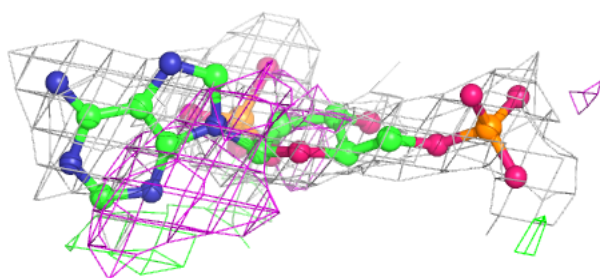
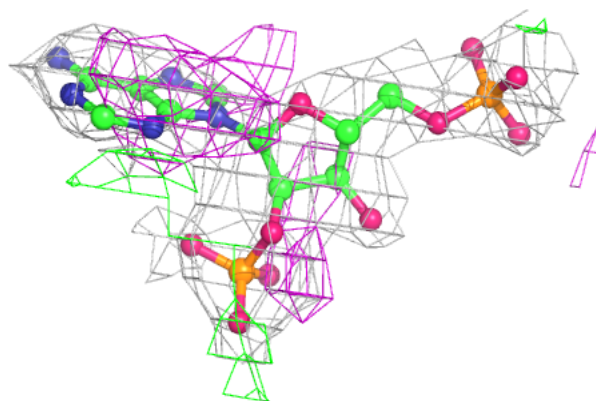
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



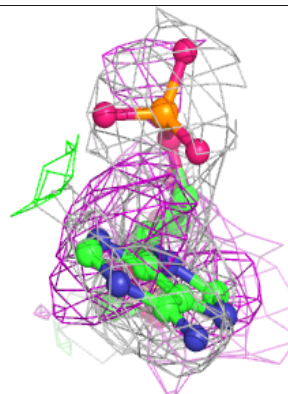
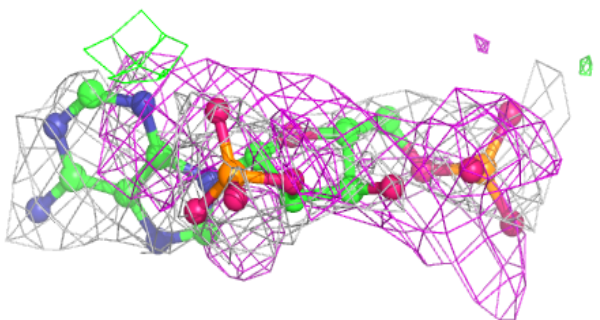
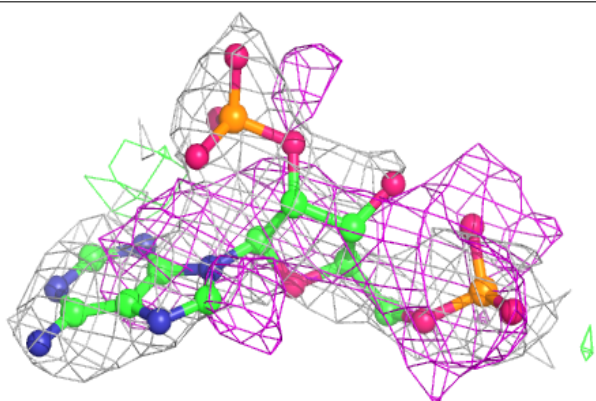


**Electron density around A2P D 1923:**

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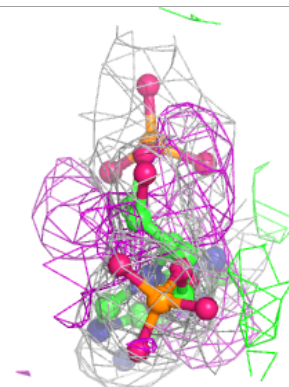
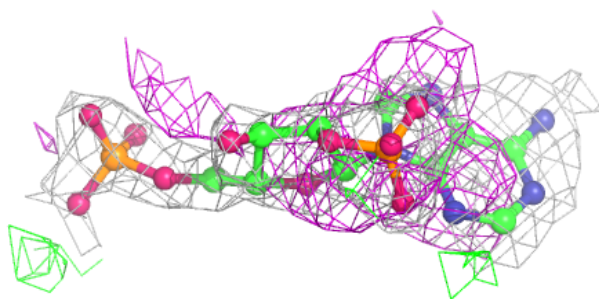
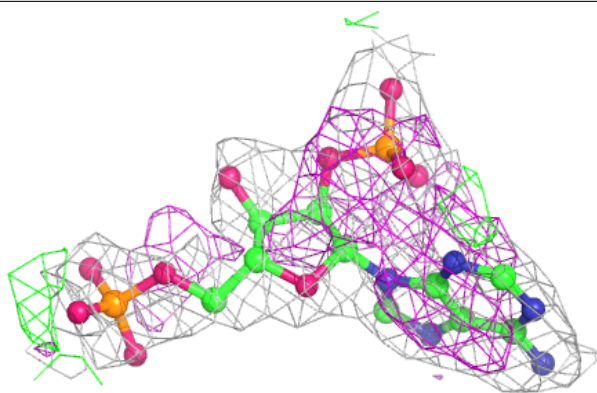
**Electron density around A2P E 1917:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

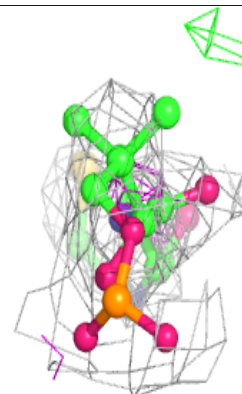
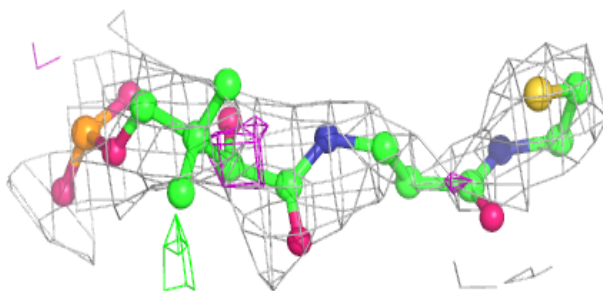
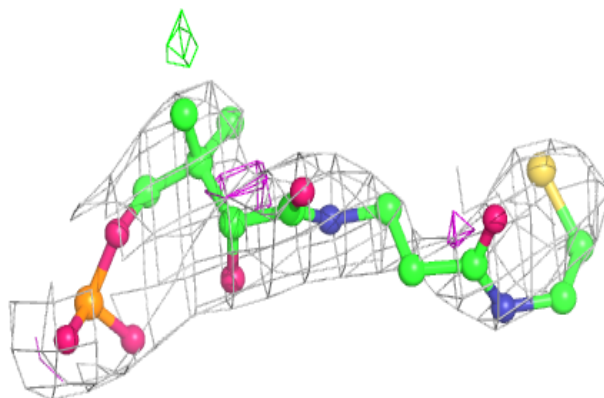


**Electron density around A2P C 1917:**

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and green (positive)

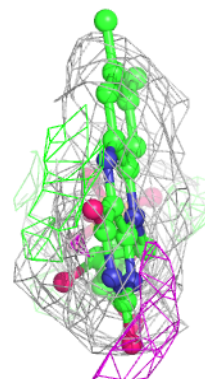
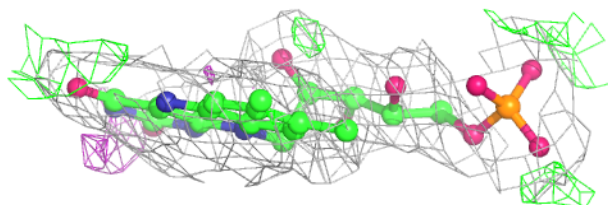
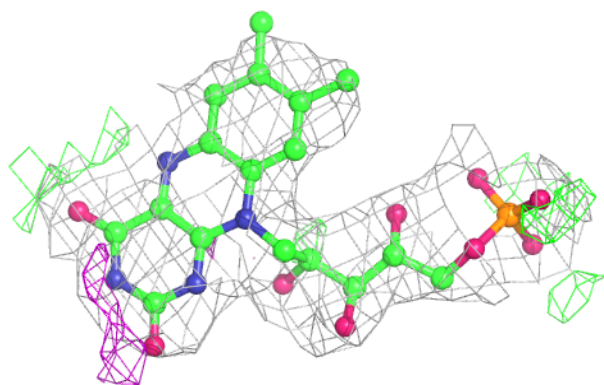
**Electron density around PNS B 1901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

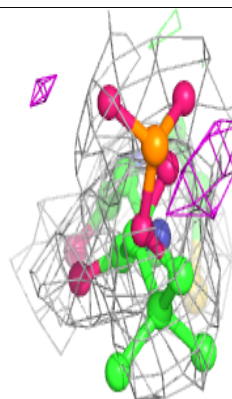
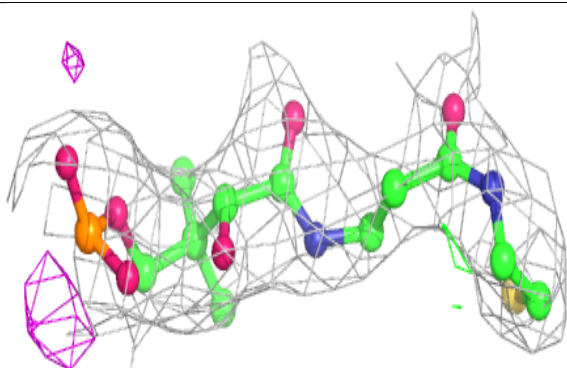
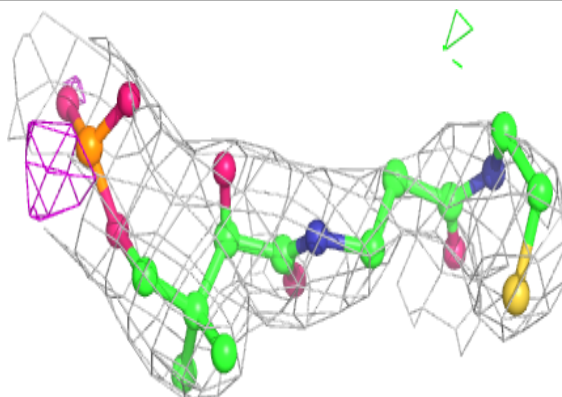


**Electron density around FMN K 2101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

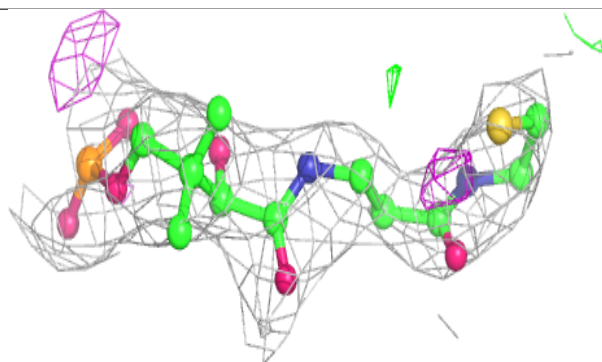
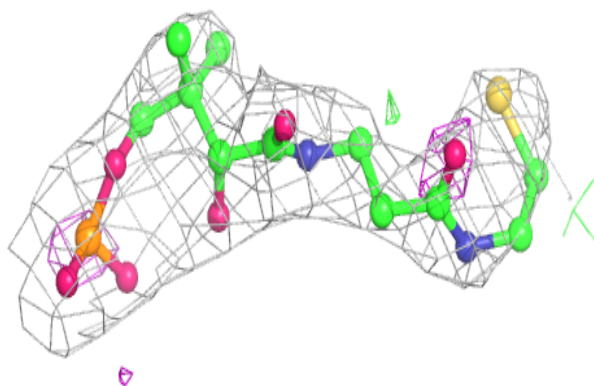
**Electron density around PNS F 1901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

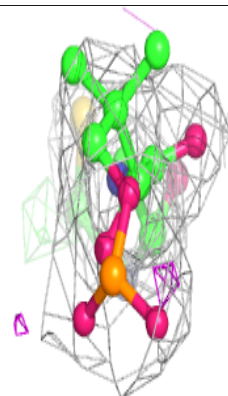
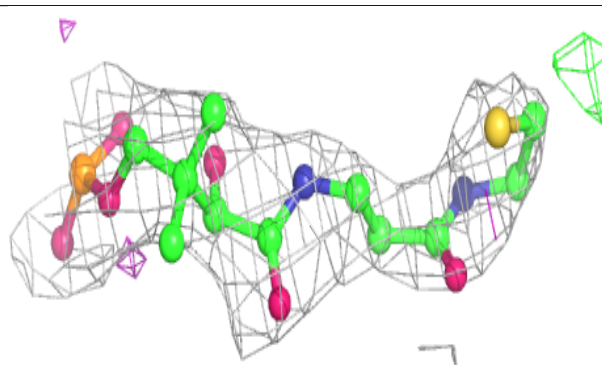
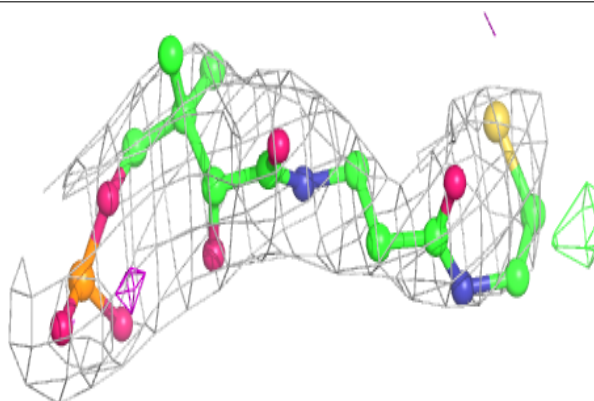


**Electron density around PNS C 1901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PNS E 1901:**

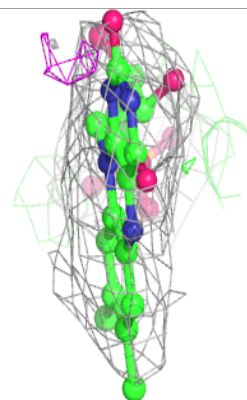
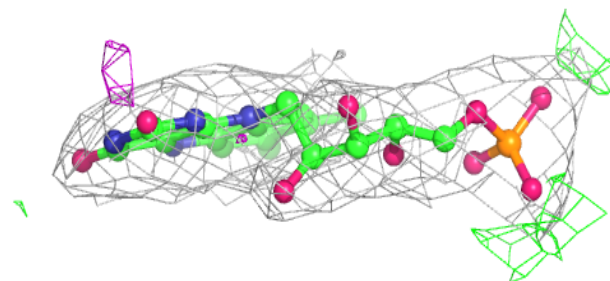
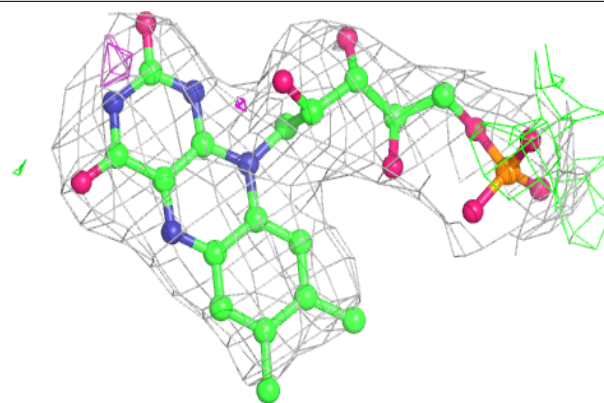
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



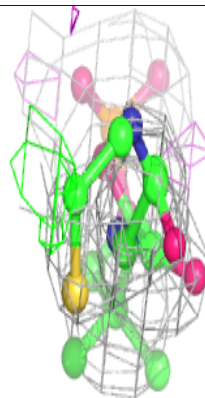
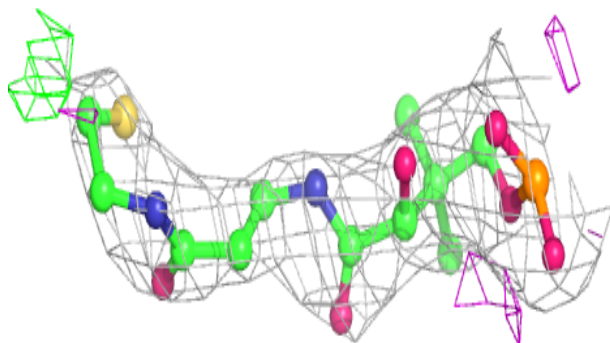
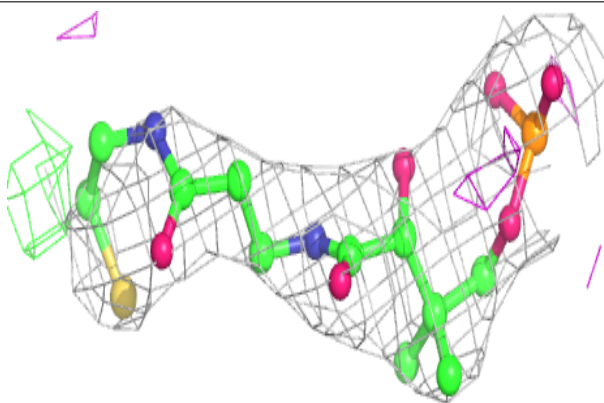


**Electron density around FMN I 2101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

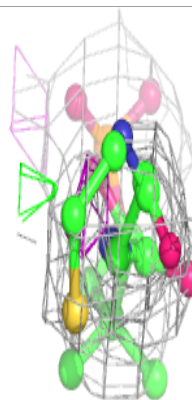
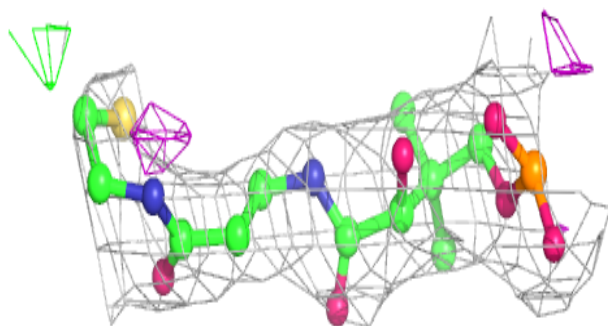
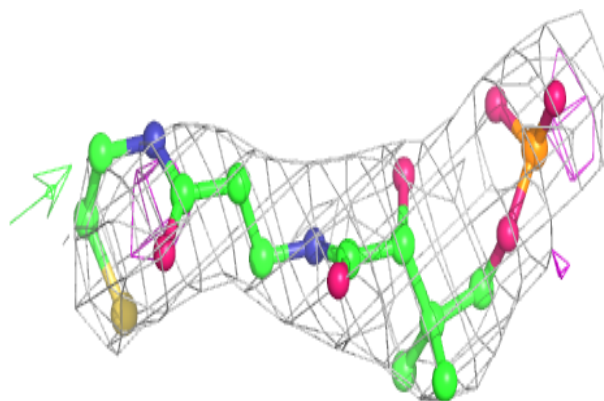
**Electron density around PNS D 1901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

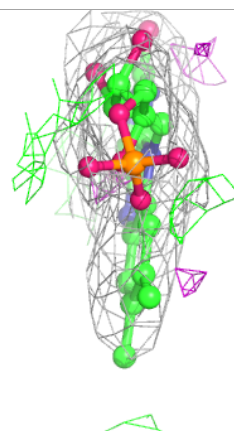
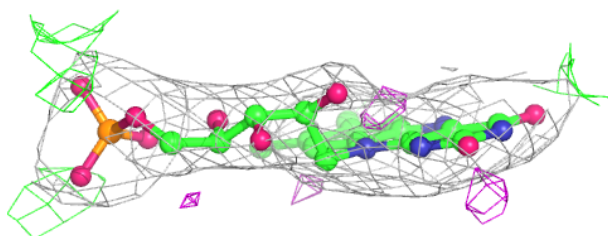
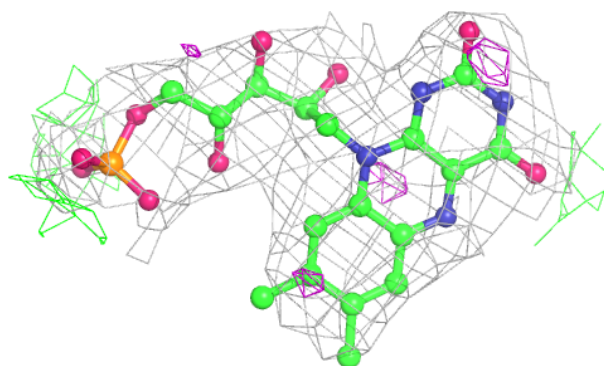


**Electron density around PNS A 1901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

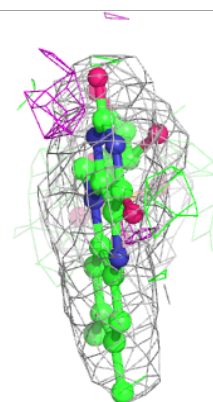
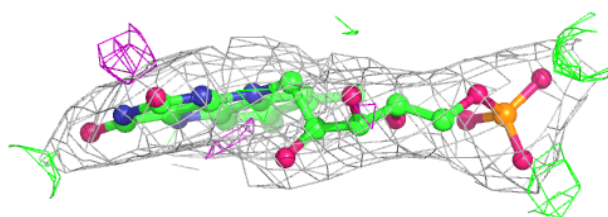
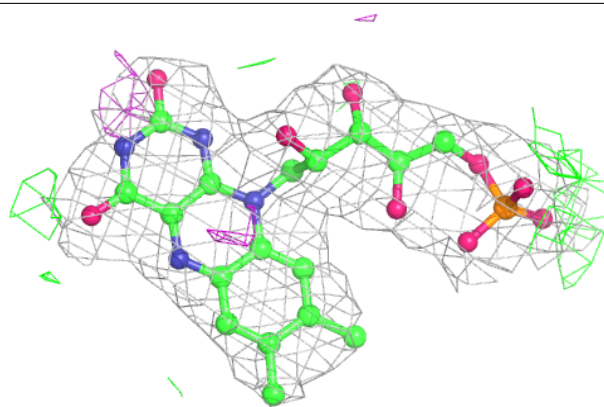
**Electron density around FMN L 2101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

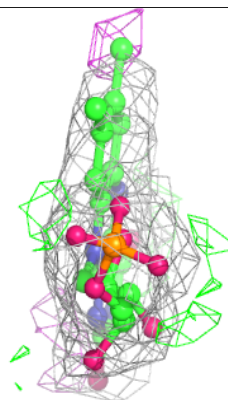
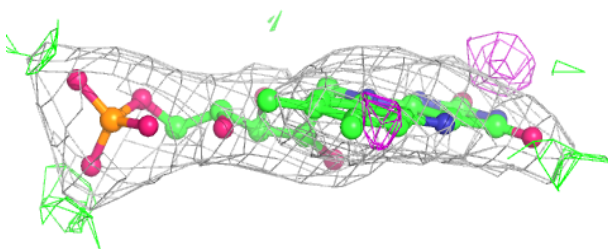
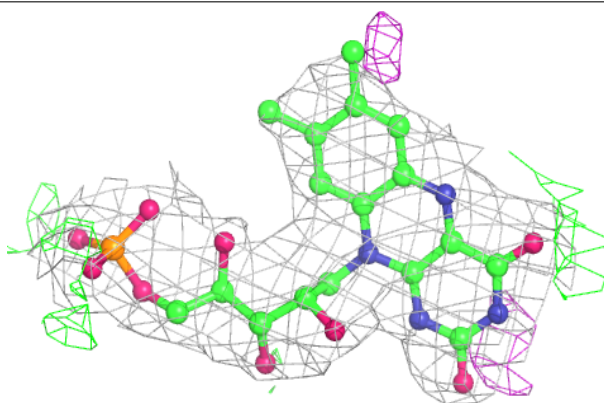


**Electron density around FMN J 2101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

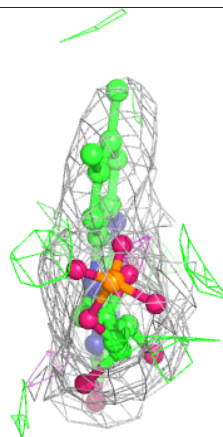
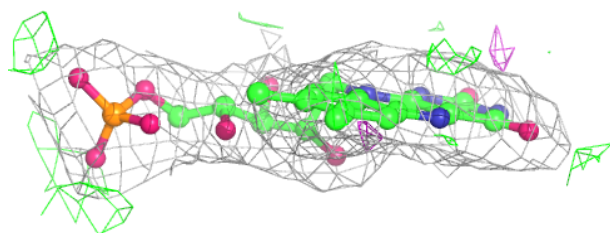
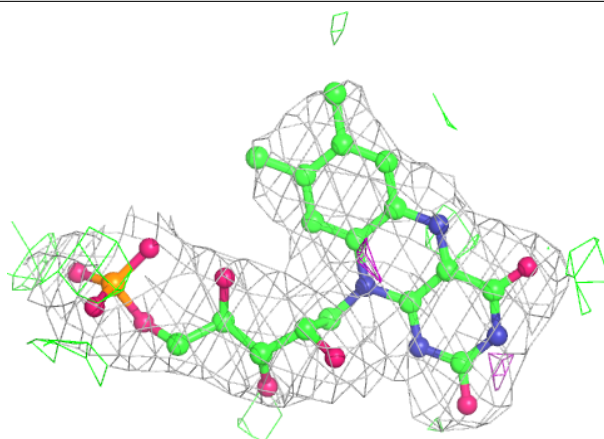
**Electron density around FMN G 2101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN H 2101:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.